U.S. DEPARTMENT OF COMMERCE
Patent and Trademark Office

SEARCH REQUEST FORM

58362

Requestor's Name: Bent

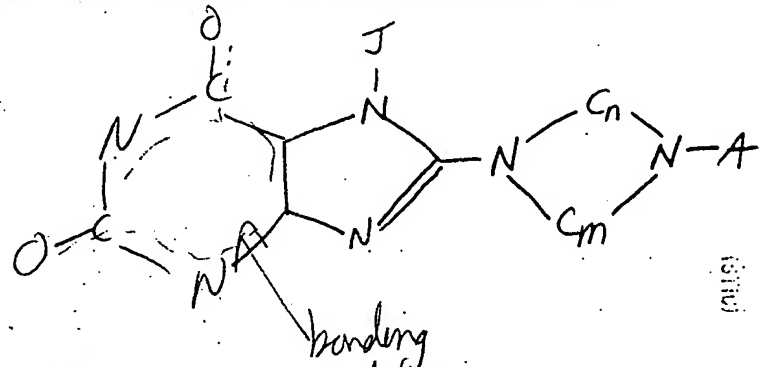
Serial Number: 09/935,146

Date: 1/15/02 Phone: 4478 4D25

Art Unit: 1624 4E12 MSG

Search Topic:

Please write a detailed statement of search topic. Describe specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples or relevant citations, authors keywords, etc., if known. For sequences, please attach a copy of the sequence. You may include a copy of the broadest and/or most relevant claim(s).



n, @ = 1-3

m = 2-4

A = H/CH3

J = C (A/Hal) (H/C@/Hal) H/C

MARY

If you get >10 hits, leave J open (and note tautomer conform).

6.19.24 4.45 99 683

8.47 $ 24-34 14

STAFF USE ONLY

Date completed: 1/28

Searcher: Mary

Terminal time:

Elapsed time:

CPU time:

Total time: 23

Number of Searches:

Number of Databases:

Search Site

- STIC
- CM-1
- Pre-S

Type of Search

- N.A. Sequence
- A.A. Sequence
- 1 Structure
- Bibliographic

Vendors

- IG Suite
- 623.99 STN
- Dialog
- APS
- Geninfo
- SDC
- DARC/Questel
- Other

Beuch
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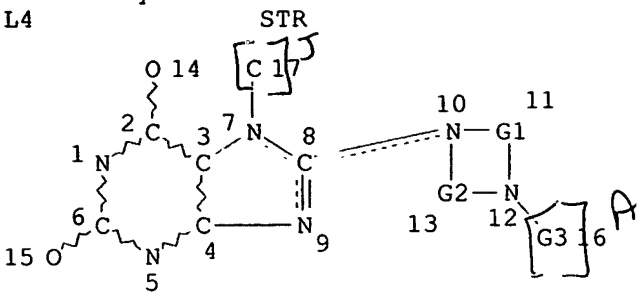
L4 STR



REP G1=(1-3) C
REP G2=(2-4) C
VAR G3=H/ME
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

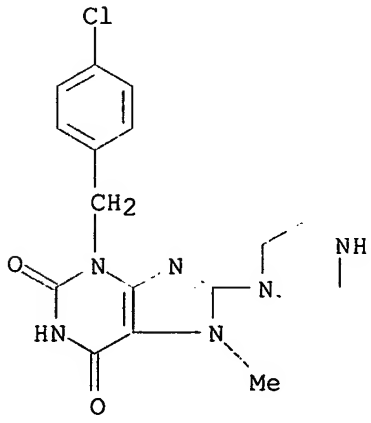
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE
L5 168 SEA FILE=REGISTRY SSS FUL L4

100.0% PROCESSED 706 ITERATIONS 168 ANSWERS
SEARCH TIME: 00.00.15

=> d 1-168 ide cbib abs;fil caol;s l5

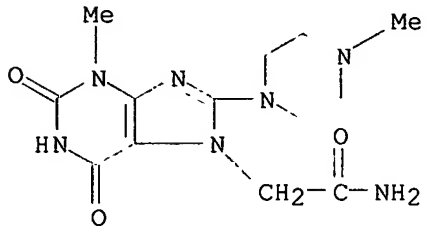
L5 ANSWER 1 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 382620-25-9 REGISTRY
CN 1H-Purine-2,6-dione, 3-[(4-chlorophenyl)methyl]-3,7-dihydro-7-methyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H19 Cl N6 O2
SR Chemical Library



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

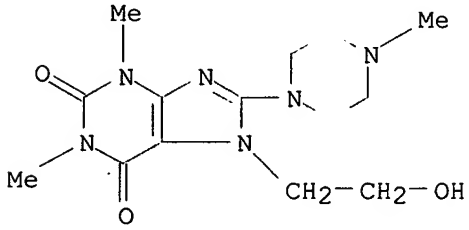
Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 2 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 378217-46-0 REGISTRY
CN 7H-Purine-7-acetamide, 1,2,3,6-tetrahydro-3-methyl-8-(4-methyl-1-piperazinyl)-2,6-dioxo- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H19 N7 O3
SR Chemical Library



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

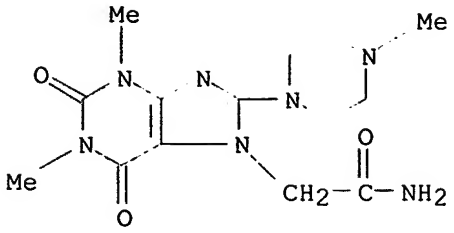
L5 ANSWER 3 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 378209-44-0 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-(2-hydroxyethyl)-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H22 N6 O3
SR Chemical Library



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

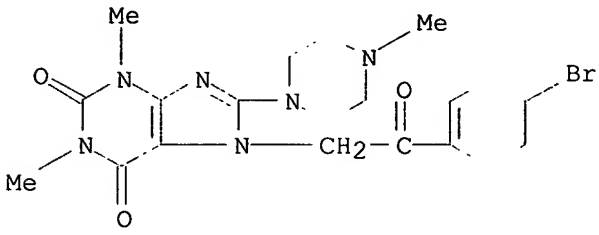
L5 ANSWER 4 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 378206-26-9 REGISTRY
CN 7H-Purine-7-acetamide, 1,2,3,6-tetrahydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)-2,6-dioxo- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H21 N7 O3
SR Chemical Library

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 5 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 378205-13-1 REGISTRY
CN 1H-Purine-2,6-dione, 7-[2-(4-bromophenyl)-2-oxoethyl]-3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H23 Br N6 O3
SR Chemical Library



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L5 ANSWER 6 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 377063-97-3 REGISTRY
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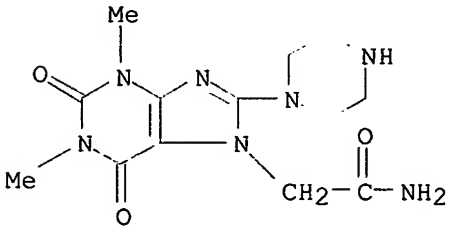
SR Chemical Library

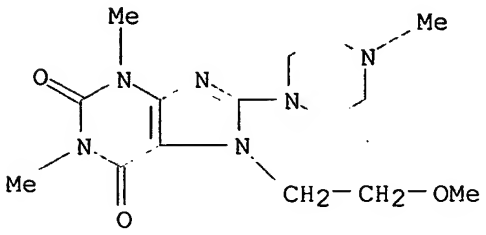


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 7 OF 168 REGISTRY COPYRIGHT 2002 ACS

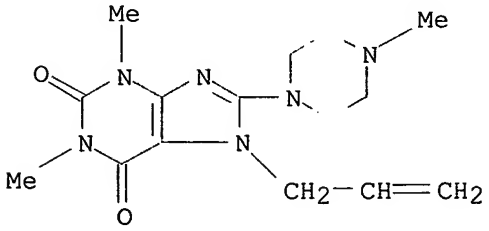
Searched by: Mary Hale 308-4258 CM-1 12D16

RN 377058-48-5 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-(2-methoxyethyl)-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H24 N6 O3
SR Chemical Library



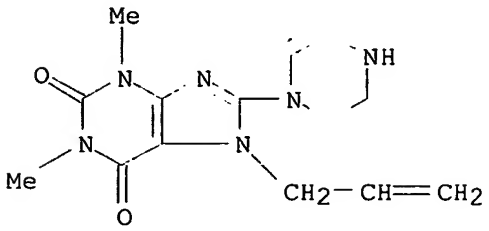
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 8 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 377057-95-9 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)-7-(2-propenyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H22 N6 O2
SR Chemical Library



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 9 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 376624-10-1 REGISTRY
CN INDEX NAME NOT YET ASSIGNED
FS 3D CONCORD
MF C14 H20 N6 O2
SR Chemical Library



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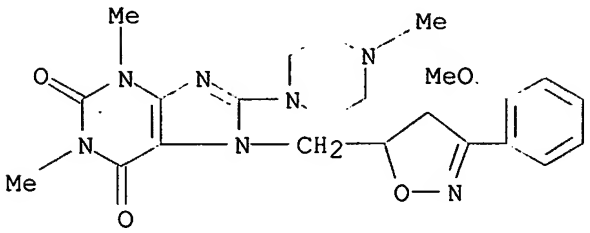
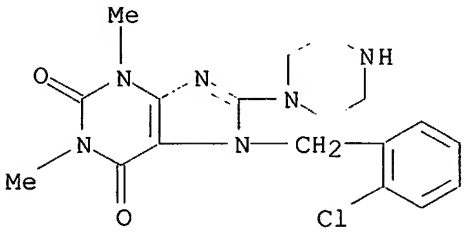
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 10 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 376621-43-1 REGISTRY
CN INDEX NAME NOT YET ASSIGNED
FS 3D CONCORD
MF C23 H29 N7 O4
SR Chemical Library



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

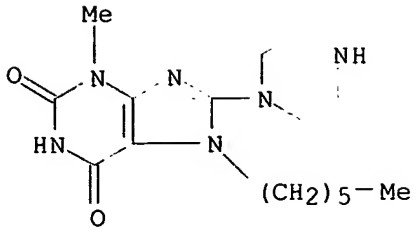
L5 ANSWER 11 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 374612-08-5 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(2-chlorophenyl)methyl]-3,7-dihydro-1,3-dimethyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
MF C18 H21 Cl N6 O2
SR Chemical Library



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 12 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 371927-37-6 REGISTRY
CN 1H-Purine-2,6-dione, 7-hexyl-3,7-dihydro-3-methyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H26 N6 O2
SR Chemical Library

Searched by: Mary Hale 308-4258 CM-1 12D16



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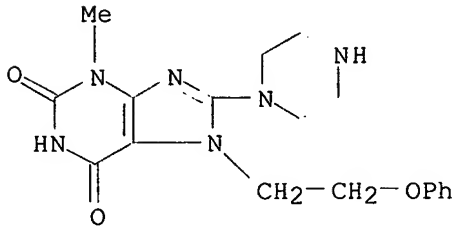
L5 ANSWER 13 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 368432-84-2 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-(2-phenoxyethyl)-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H22 N6 O3
SR Chemical Library



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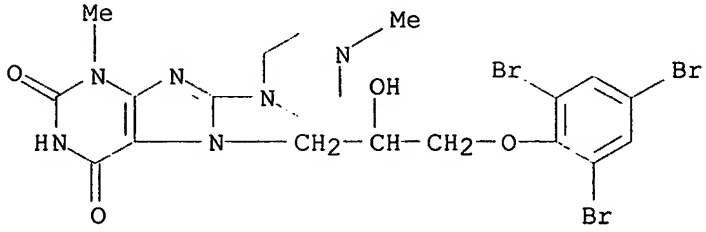
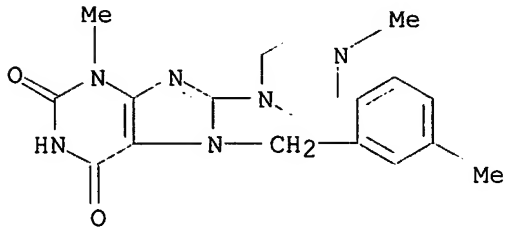
L5 ANSWER 14 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 364371-37-9 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-3-(2,4,6-tribromophenoxy)propyl]-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H23 Br3 N6 O4
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

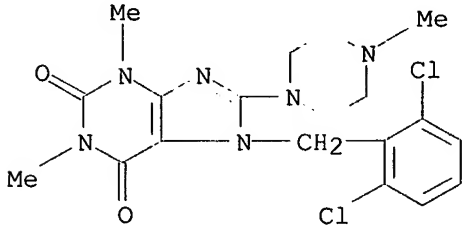
Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 15 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 361174-74-5 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-[(3-methylphenyl)methyl]-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H24 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

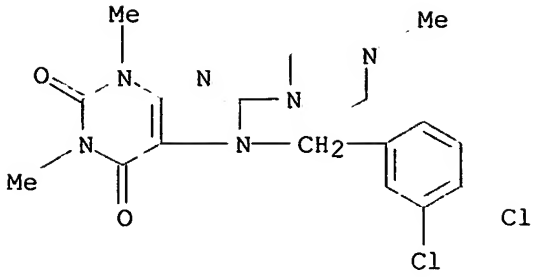
L5 ANSWER 16 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 359909-06-1 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(2,6-dichlorophenyl)methyl]-3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
MF C19 H22 Cl2 N6 O2
SR Chemical Library



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

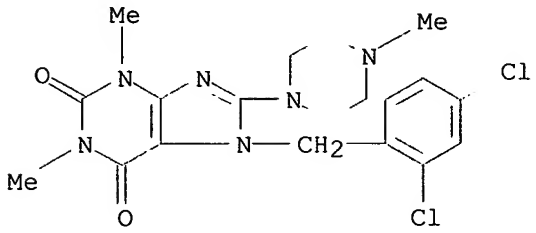
L5 ANSWER 17 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 359908-69-3 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(3,4-dichlorophenyl)methyl]-3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H22 Cl2 N6 O2
SR Chemical Library

Searched by: Mary Hale 308-4258 CM-1 12D16



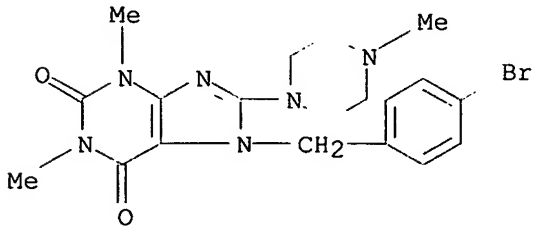
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 18 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 359908-14-8 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(2,4-dichlorophenyl)methyl]-3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
MF C19 H22 Cl2 N6 O2
SR Chemical Library



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

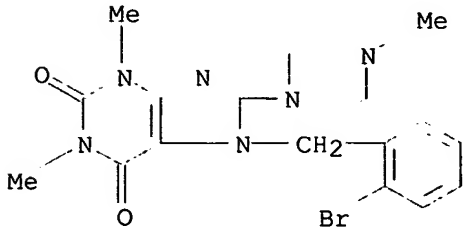
L5 ANSWER 19 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 359907-82-7 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(4-bromophenyl)methyl]-3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H23 Br N6 O2
SR Chemical Library



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 20 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 359904-67-9 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(2-bromophenyl)methyl]-3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
MF C19 H23 Br N6 O2
SR Chemical Library



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 21 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 359903-52-9 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(2-fluorophenyl)methyl]-3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
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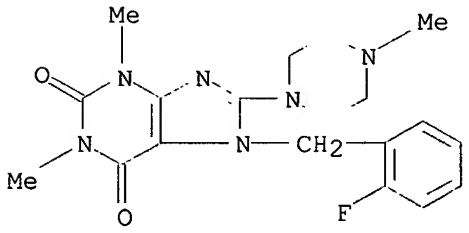
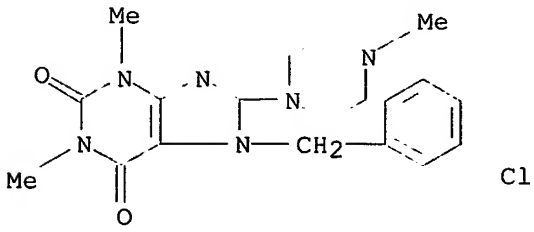
SR Chemical Library



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

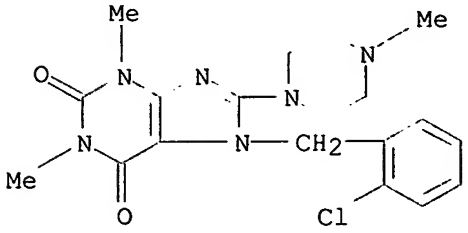
L5 ANSWER 22 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 359902-95-7 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(3-chlorophenyl)methyl]-3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H23 Cl N6 O2
SR Chemical Library



Searched by: Mary Hale 308-4258 CM-1 12D16

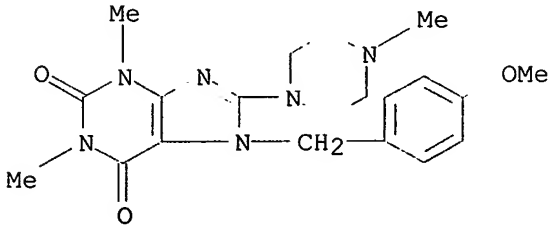
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 23 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 359902-76-4 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(2-chlorophenyl)methyl]-3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
MF C19 H23 Cl N6 O2
SR Chemical Library



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

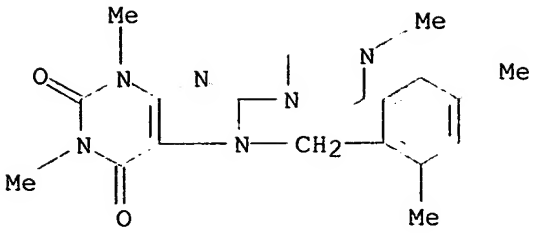
L5 ANSWER 24 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 359902-48-0 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[(4-methoxyphenyl)methyl]-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H26 N6 O3
SR Chemical Library



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 25 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 359902-17-3 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(2,4-dimethylphenyl)methyl]-3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H28 N6 O2
SR Chemical Library

Searched by: Mary Hale 308-4258 CM-1 12D16



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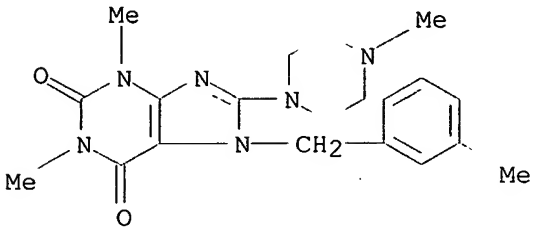
L5 ANSWER 26 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 359901-61-4 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-7-[(3-methylphenyl)methyl]-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H26 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



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L5 ANSWER 27 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 359698-07-0 REGISTRY
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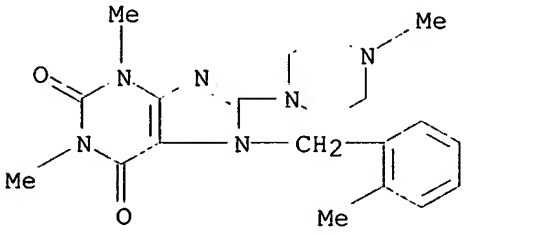
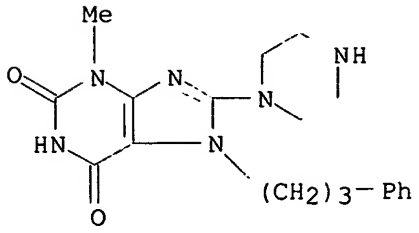
FS 3D CONCORD
MF C20 H26 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

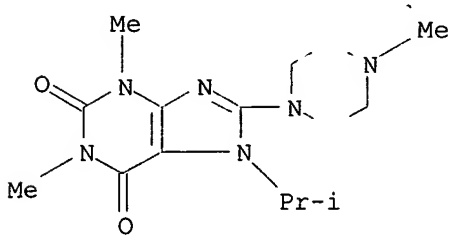
Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 28 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 353255-08-0 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-(3-phenylpropyl)-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H24 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

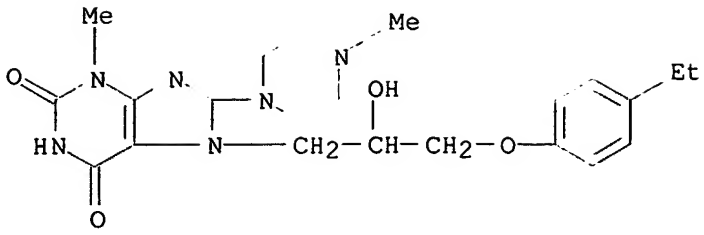
L5 ANSWER 29 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 335403-41-3 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-7-(1-methylethyl)-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H24 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

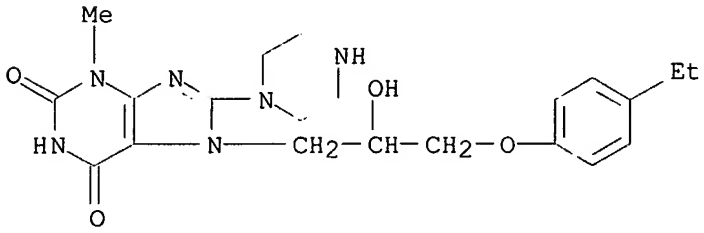
L5 ANSWER 30 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 335403-14-0 REGISTRY
CN 1H-Purine-2,6-dione, 7-[3-(4-ethylphenoxy)-2-hydroxypropyl]-3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C22 H30 N6 O4
SR Chemical Library
LC STN Files: CHEMCATS

Searched by: Mary Hale 308-4258 CM-1 12D16



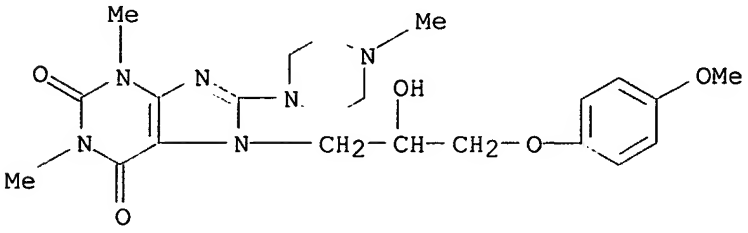
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 31 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 335403-13-9 REGISTRY
CN 1H-Purine-2,6-dione, 7-[3-(4-ethylphenoxy)-2-hydroxypropyl]-3,7-dihydro-3-methyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H28 N6 O4
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

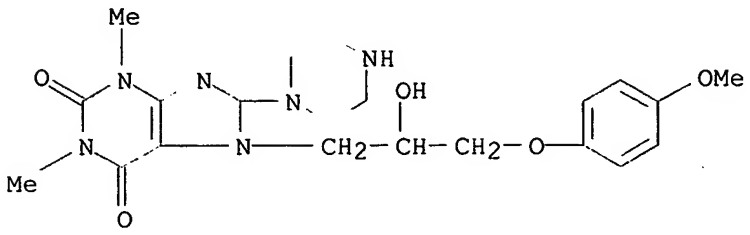
L5 ANSWER 32 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 333755-40-1 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-3-(4-methoxyphenoxy)propyl]-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C22 H30 N6 O5
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

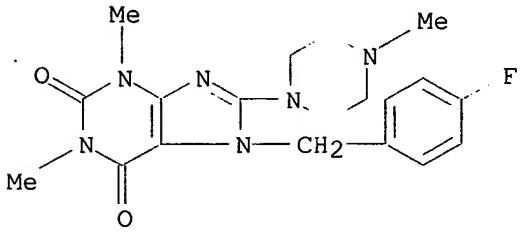
Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 33 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 333755-39-8 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-3-(4-methoxyphenoxy)propyl]-1,3-dimethyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H28 N6 O5
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

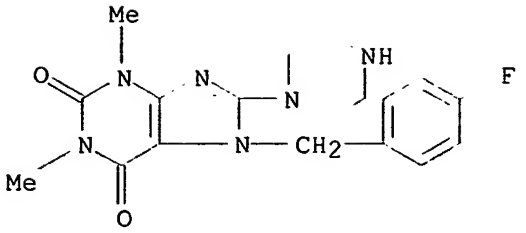
L5 ANSWER 34 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 333755-23-0 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(4-fluorophenyl)methyl]-3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H23 F N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

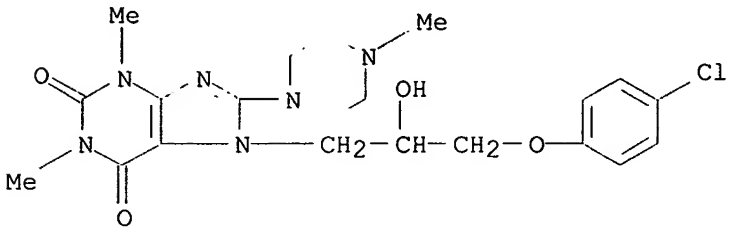
L5 ANSWER 35 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 333755-22-9 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(4-fluorophenyl)methyl]-3,7-dihydro-1,3-dimethyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H21 F N6 O2
SR Chemical Library
LC STN Files: CHEMCATS

Searched by: Mary Hale 308-4258 CM-1 12D16



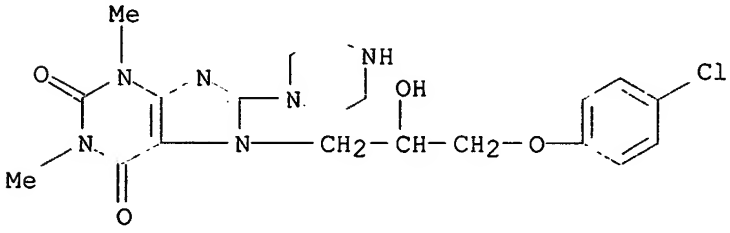
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 36 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 333305-43-4 REGISTRY
CN 1H-Purine-2,6-dione, 7-[3-(4-chlorophenoxy)-2-hydroxypropyl]-3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H27 Cl N6 O4
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

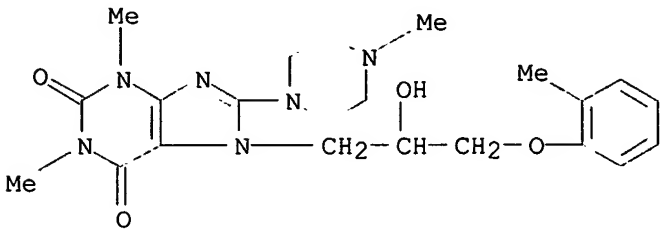
L5 ANSWER 37 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 333305-42-3 REGISTRY
CN 1H-Purine-2,6-dione, 7-[3-(4-chlorophenoxy)-2-hydroxypropyl]-3,7-dihydro-1,3-dimethyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H25 Cl N6 O4
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

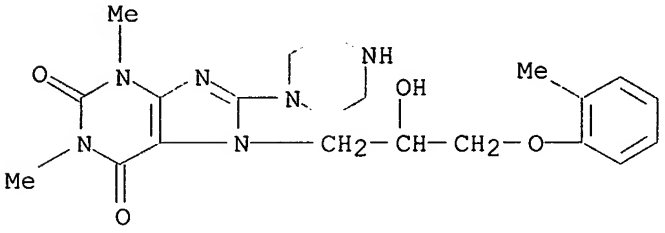
Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 38 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 333305-37-6 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-3-(2-methylphenoxy)propyl]-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C22 H30 N6 O4
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

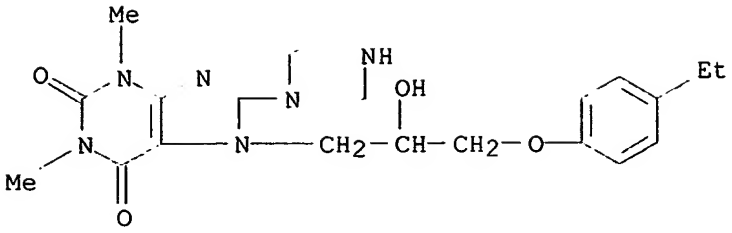
L5 ANSWER 39 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 333305-36-5 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-3-(2-methylphenoxy)propyl]-1,3-dimethyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H28 N6 O4
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

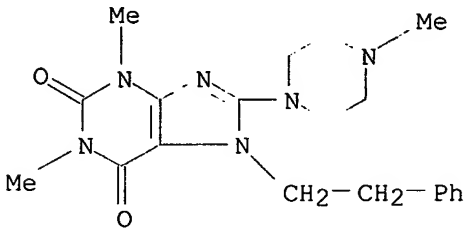
L5 ANSWER 40 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 333305-27-4 REGISTRY
CN 1H-Purine-2,6-dione, 7-[3-(4-ethylphenoxy)-2-hydroxypropyl]-3,7-dihydro-1,3-dimethyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C22 H30 N6 O4
SR Chemical Library
LC STN Files: CHEMCATS

Searched by: Mary Hale 308-4258 CM-1 12D16



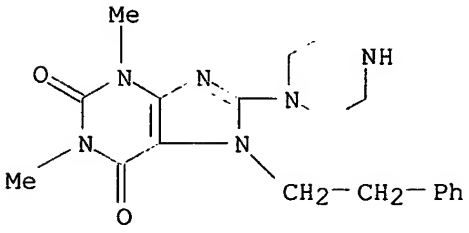
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 41 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 333305-06-9 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)-7-(2-phenylethyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H26 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

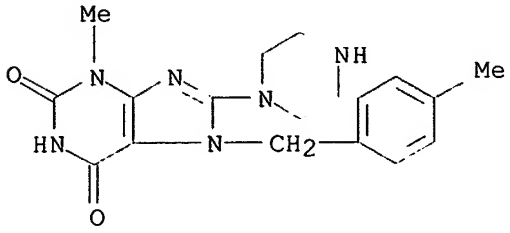
L5 ANSWER 42 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 333305-05-8 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-7-(2-phenylethyl)-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H24 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

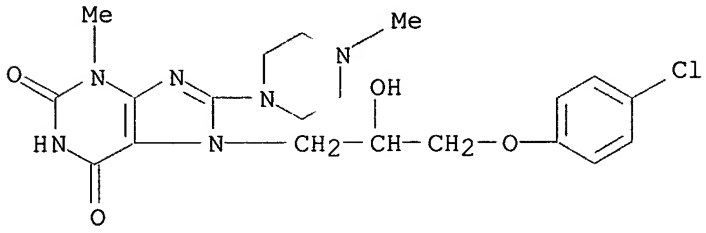
Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 43 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332905-08-5 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-[(4-methylphenyl)methyl]-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H22 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

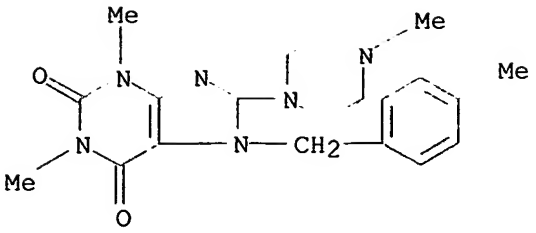
L5 ANSWER 44 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332904-83-3 REGISTRY
CN 1H-Purine-2,6-dione, 7-[3-(4-chlorophenoxy)-2-hydroxypropyl]-3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H25 Cl N6 O4
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

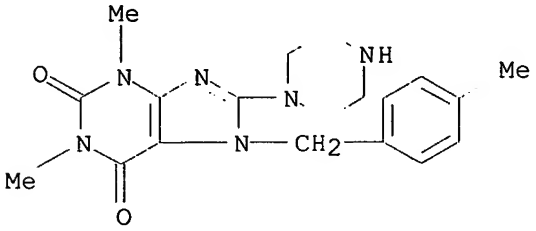
L5 ANSWER 45 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332904-77-5 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-7-[(4-methylphenyl)methyl]-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H26 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS

Searched by: Mary Hale 308-4258 CM-1 12D16



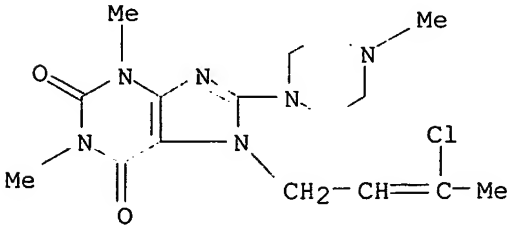
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 46 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332904-76-4 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-7-[(4-methylphenyl)methyl]-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H24 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

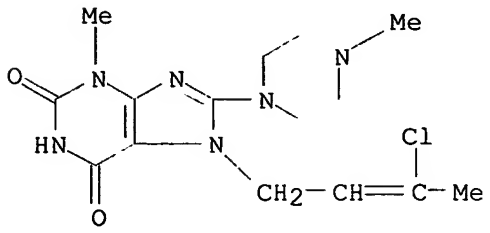
L5 ANSWER 47 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332897-97-9 REGISTRY
CN 1H-Purine-2,6-dione, 7-(3-chloro-2-butenyl)-3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H23 Cl N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

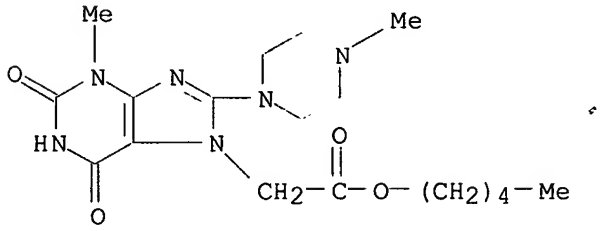
Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 48 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332897-96-8 REGISTRY
CN 1H-Purine-2,6-dione, 7-(3-chloro-2-butenyl)-3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H21 Cl N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

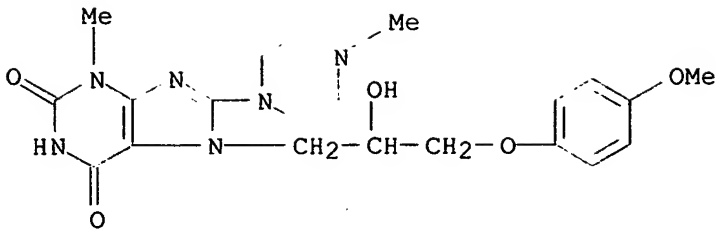
L5 ANSWER 49 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332384-43-7 REGISTRY
CN 7H-Purine-7-acetic acid, 1,2,3,6-tetrahydro-3-methyl-8-(4-methyl-1-piperazinyl)-2,6-dioxo-, pentyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H28 N6 O4
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

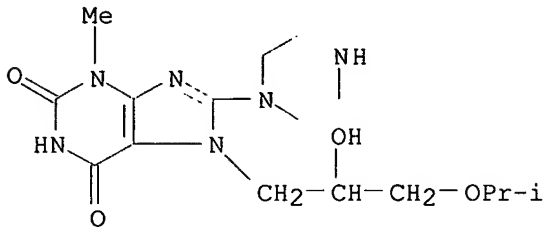
L5 ANSWER 50 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332384-42-6 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-3-(4-methoxyphenoxy)propyl]-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H28 N6 O5
SR Chemical Library
LC STN Files: CHEMCATS

Searched by: Mary Hale 308-4258 CM-1 12D16



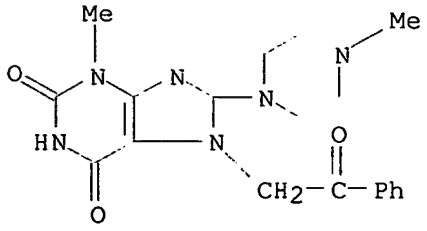
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 51 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332384-40-4 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-3-(1-methylethoxy)propyl]-3-methyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H26 N6 O4
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

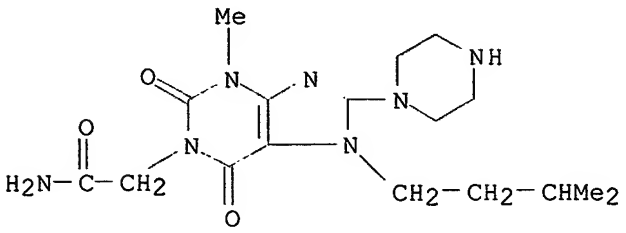
L5 ANSWER 52 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332384-28-8 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)-7-(2-oxo-2-phenylethyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H22 N6 O3
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

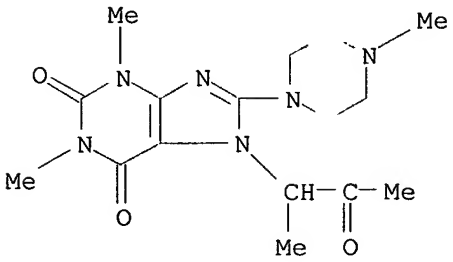
Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 53 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332151-03-8 REGISTRY
CN 1H-Purine-1-acetamide, 2,3,6,7-tetrahydro-3-methyl-7-(3-methylbutyl)-2,6-dioxo-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H27 N7 O3
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

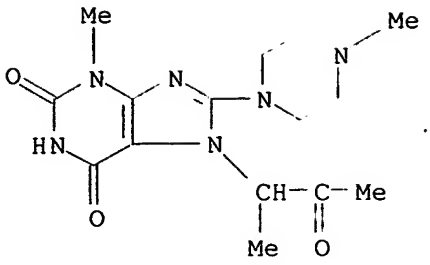
L5 ANSWER 54 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332103-78-3 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-7-(1-methyl-2-oxopropyl)-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H24 N6 O3
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

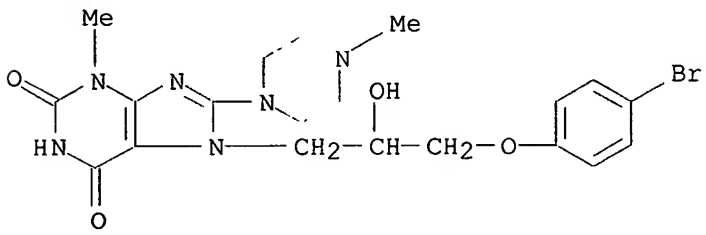
L5 ANSWER 55 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332103-77-2 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-(1-methyl-2-oxopropyl)-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H22 N6 O3
SR Chemical Library
LC STN Files: CHEMCATS

Searched by: Mary Hale 308-4258 CM-1 12D16



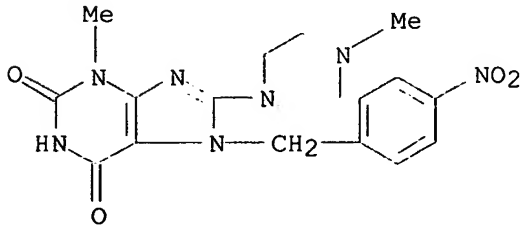
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 56 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332103-75-0 REGISTRY
CN 1H-Purine-2,6-dione, 7-[3-(4-bromophenoxy)-2-hydroxypropyl]-3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H25 Br N6 O4
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

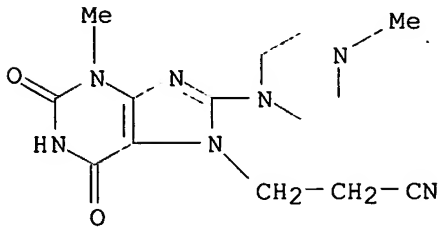
L5 ANSWER 57 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332103-66-9 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)-7-[(4-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H21 N7 O4
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

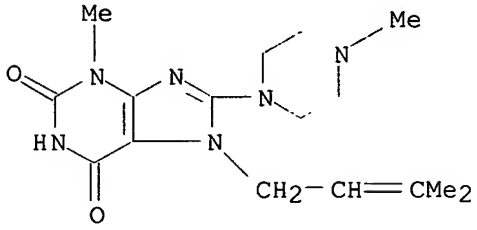
Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 58 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332103-65-8 REGISTRY
CN 7H-Purine-7-propanenitrile, 1,2,3,6-tetrahydro-3-methyl-8-(4-methyl-1-piperazinyl)-2,6-dioxo- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H19 N7 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

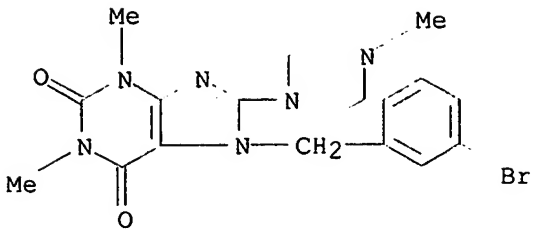
L5 ANSWER 59 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332103-64-7 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-(3-methyl-2-butenyl)-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H24 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

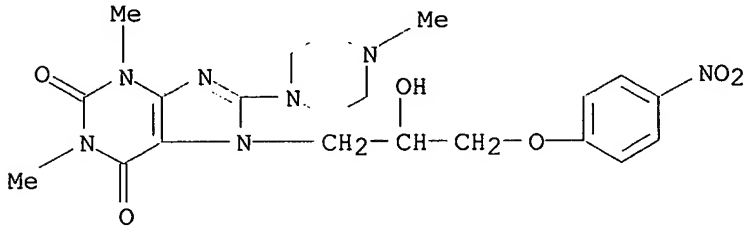
L5 ANSWER 60 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332103-62-5 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(3-bromophenyl)methyl]-3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H23 Br N6 O2
SR Chemical Library
LC STN Files: CHEMCATS

Searched by: Mary Hale 308-4258 CM-1 12D16



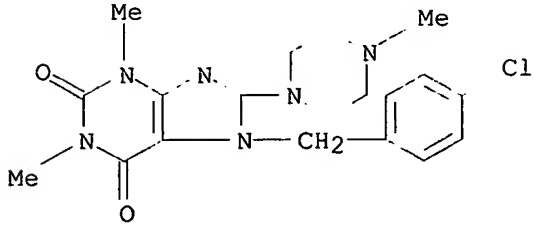
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 61 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332103-61-4 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-3-(4-nitrophenoxy)propyl]-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H27 N7 O6
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

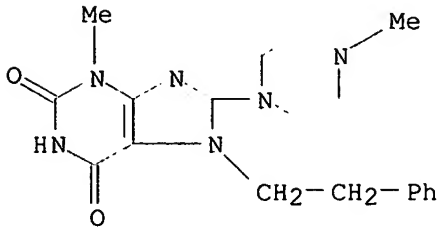
L5 ANSWER 62 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332103-60-3 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(4-chlorophenyl)methyl]-3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H23 Cl N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

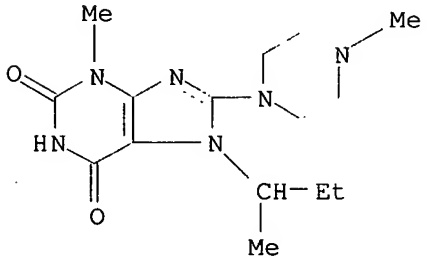
Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 63 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332103-59-0 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)-7-(2-phenylethyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H24 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

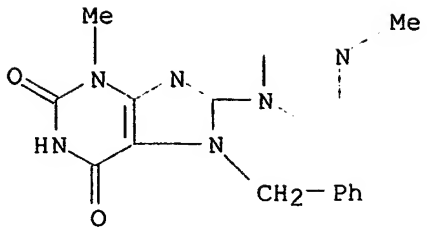
L5 ANSWER 64 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332103-58-9 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)-7-(1-methylpropyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H24 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

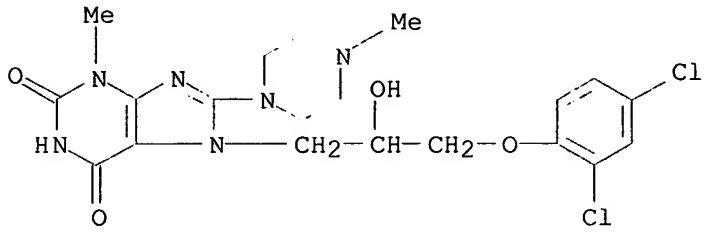
L5 ANSWER 65 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332103-57-8 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H22 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS

Searched by: Mary Hale 308-4258 CM-1 12D16



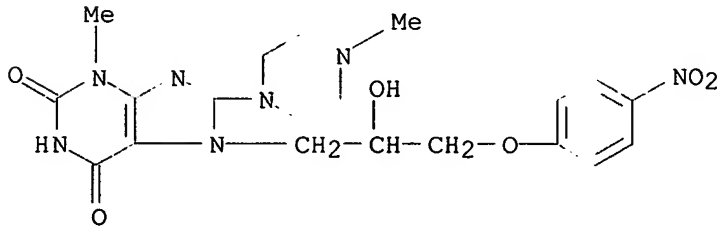
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 66 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332103-56-7 REGISTRY
CN 1H-Purine-2,6-dione, 7-[3-(2,4-dichlorophenoxy)-2-hydroxypropyl]-3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H24 Cl2 N6 O4
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

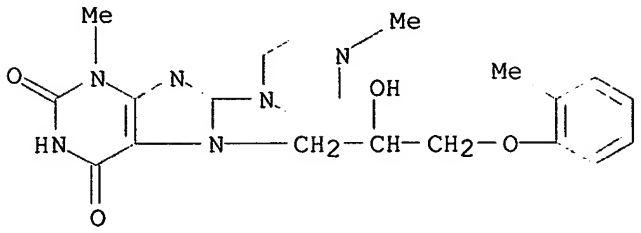
L5 ANSWER 67 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332103-55-6 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-3-(4-nitrophenoxy)propyl]-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H25 N7 O6
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

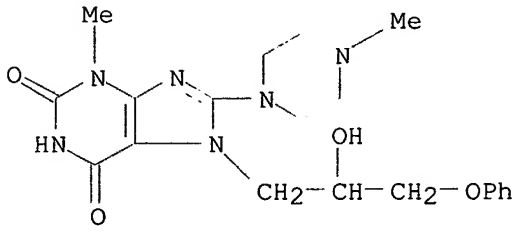
Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 68 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332103-54-5 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-3-(2-methylphenoxy)propyl]-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H28 N6 O4
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

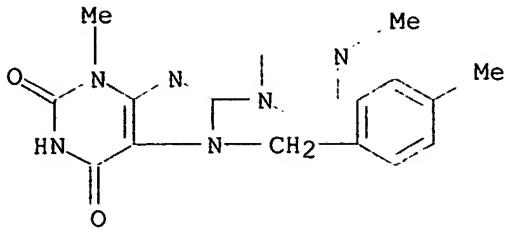
L5 ANSWER 69 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332103-53-4 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-(2-hydroxy-3-phenoxypropyl)-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H26 N6 O4
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

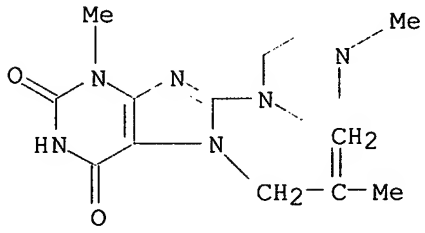
L5 ANSWER 70 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332103-52-3 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-[(4-methylphenyl)methyl]-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H24 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS

Searched by: Mary Hale 308-4258 CM-1 12D16



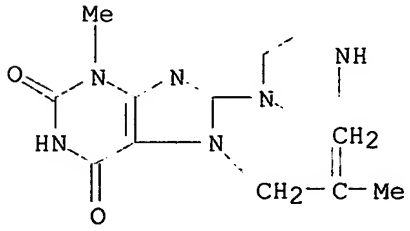
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 71 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332098-98-3 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)-7-(2-methyl-2-propenyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H22 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

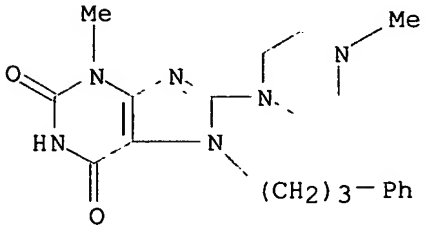
L5 ANSWER 72 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332098-96-1 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-(2-methyl-2-propenyl)-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H20 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

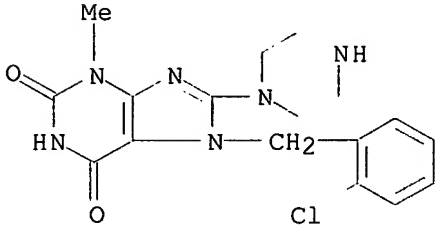
Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 73 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 332033-44-0 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)-7-(3-phenylpropyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H26 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

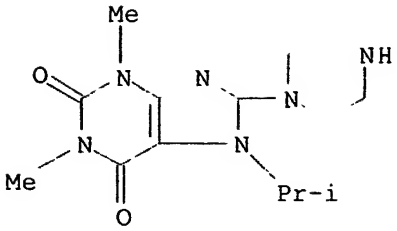
L5 ANSWER 74 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 331841-51-1 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(2-chlorophenyl)methyl]-3,7-dihydro-3-methyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
MF C17 H19 Cl N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

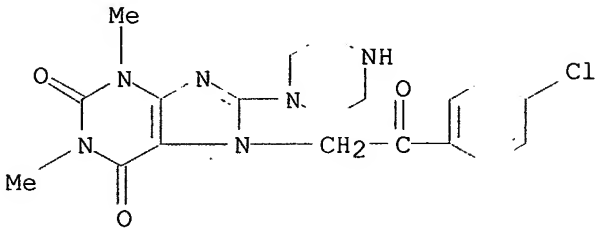
L5 ANSWER 75 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 331671-66-0 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-7-(1-methylethyl)-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H22 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS

Searched by: Mary Hale 308-4258 CM-1 12D16



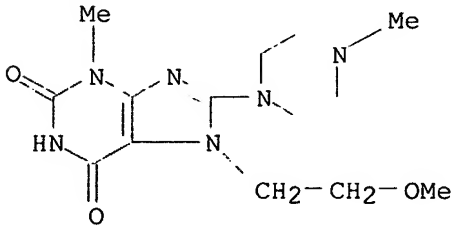
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 76 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 331671-64-8 REGISTRY
CN 1H-Purine-2,6-dione, 7-[2-(4-chlorophenyl)-2-oxoethyl]-3,7-dihydro-1,3-dimethyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H21 Cl N6 O3
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

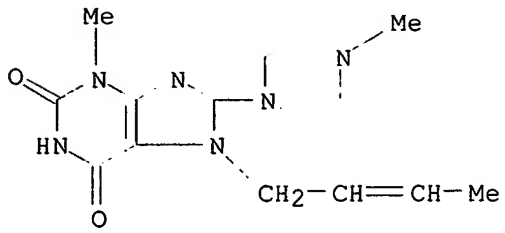
L5 ANSWER 77 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 330202-50-1 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-(2-methoxyethyl)-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H22 N6 O3
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

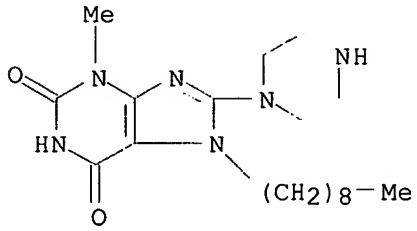
Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 78 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 330202-48-7 REGISTRY
CN 1H-Purine-2,6-dione, 7-(2-butenyl)-3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H22 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

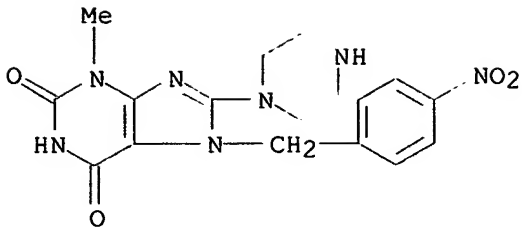
L5 ANSWER 79 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 329702-29-6 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-nonyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H32 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

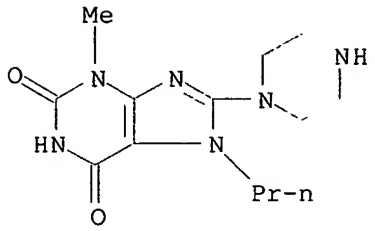
L5 ANSWER 80 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 318271-92-0 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-[(4-nitrophenyl)methyl]-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H19 N7 O4
SR Chemical Library
LC STN Files: CHEMCATS

Searched by: Mary Hale 308-4258 CM-1 12D16



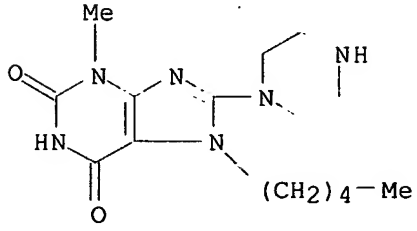
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 81 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313554-09-5 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-8-(1-piperazinyl)-7-propyl-
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H20 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

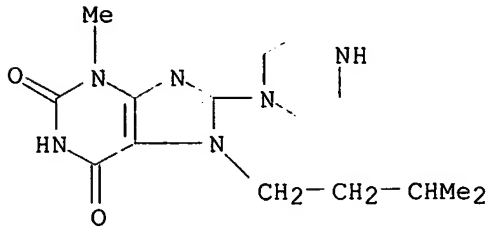
L5 ANSWER 82 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313530-91-5 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-pentyl-8-(1-piperazinyl)-
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H24 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

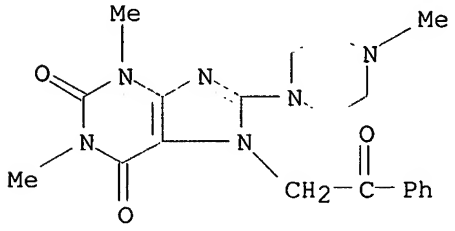
Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 83 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313530-90-4 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-(3-methylbutyl)-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H24 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

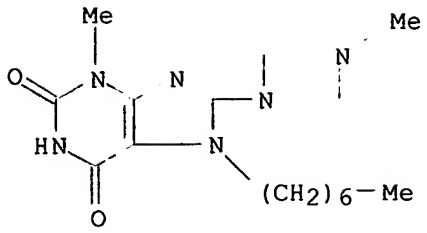
L5 ANSWER 84 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313471-57-7 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)-7-(2-oxo-2-phenylethyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H24 N6 O3
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

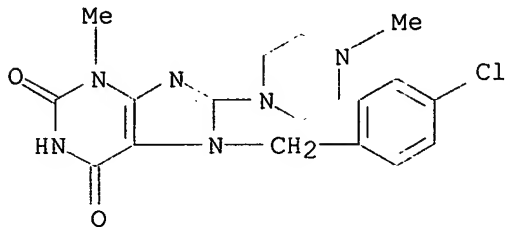
L5 ANSWER 85 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313471-56-6 REGISTRY
CN 1H-Purine-2,6-dione, 7-heptyl-3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H30 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS

Searched by: Mary Hale 308-4258 CM-1 12D16



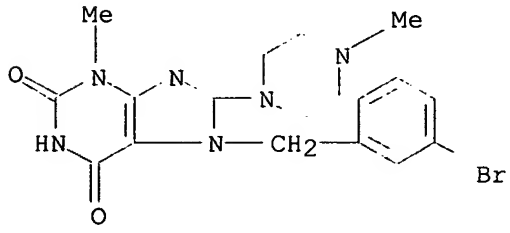
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 86 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313471-55-5 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(4-chlorophenyl)methyl]-3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H21 Cl N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

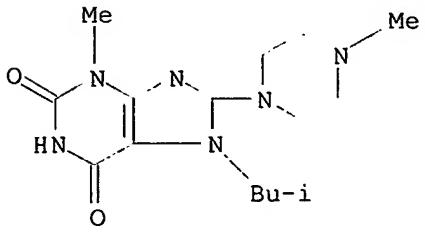
L5 ANSWER 87 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313471-54-4 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(3-bromophenyl)methyl]-3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H21 Br N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

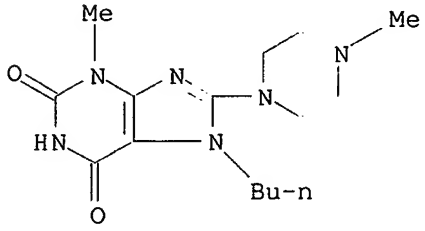
Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 88 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313471-53-3 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)-7-(2-methylpropyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H24 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

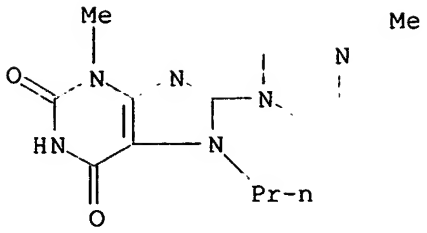
L5 ANSWER 89 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313471-52-2 REGISTRY
CN 1H-Purine-2,6-dione, 7-butyl-3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H24 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

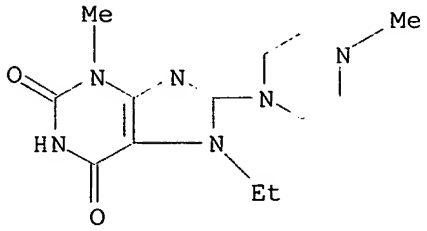
L5 ANSWER 90 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313471-50-0 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)-7-propyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H22 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS

Searched by: Mary Hale 308-4258 CM-1 12D16



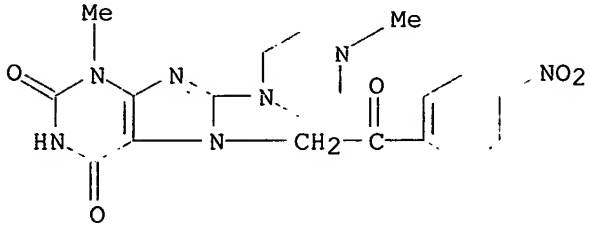
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 91 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313471-49-7 REGISTRY
CN 1H-Purine-2,6-dione, 7-ethyl-3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H20 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

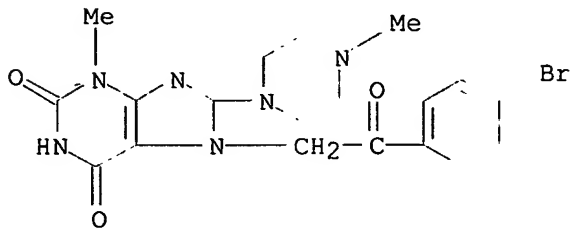
L5 ANSWER 92 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313404-89-6 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)-7-[2-(4-nitrophenyl)-2-oxoethyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H21 N7 O5
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

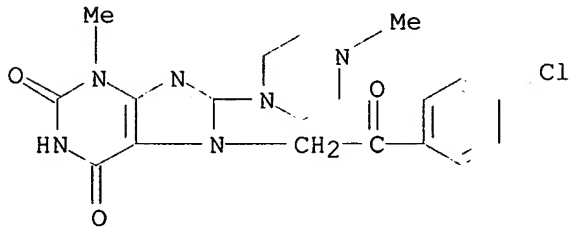
Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 93 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313404-88-5 REGISTRY
CN 1H-Purine-2,6-dione, 7-[2-(4-bromophenyl)-2-oxoethyl]-3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H21 Br N6 O3
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

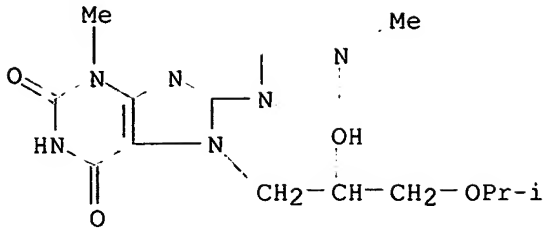
L5 ANSWER 94 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313404-64-7 REGISTRY
CN 1H-Purine-2,6-dione, 7-[2-(4-chlorophenyl)-2-oxoethyl]-3,7-dihydro-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H21 Cl N6 O3
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

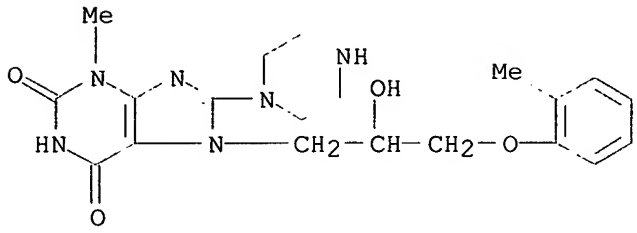
L5 ANSWER 95 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313403-94-0 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-3-(1-methylethoxy)propyl]-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H28 N6 O4
SR Chemical Library
LC STN Files: CHEMCATS

Searched by: Mary Hale 308-4258 CM-1 12D16



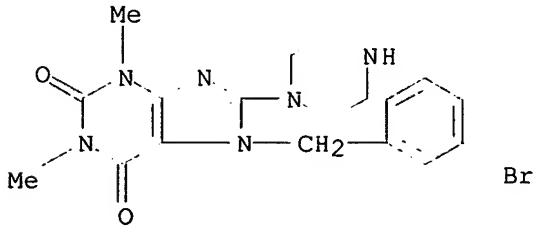
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 96 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313396-00-8 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-3-(2-methylphenoxy)propyl]-3-methyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H26 N6 O4
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

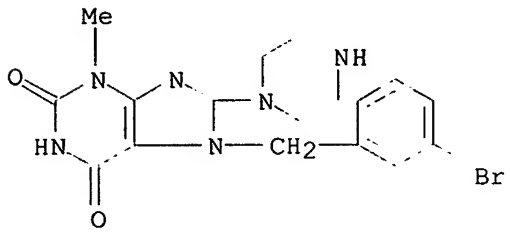
L5 ANSWER 97 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313274-01-0 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(3-bromophenyl)methyl]-3,7-dihydro-1,3-dimethyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H21 Br N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

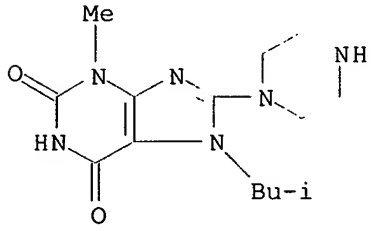
Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 98 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313274-00-9 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(3-bromophenyl)methyl]-3,7-dihydro-3-methyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H19 Br N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

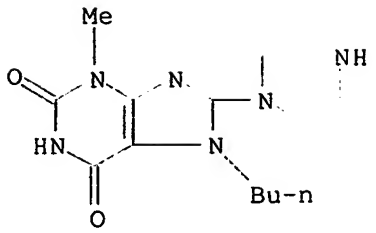
L5 ANSWER 99 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313273-71-1 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-(2-methylpropyl)-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H22 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

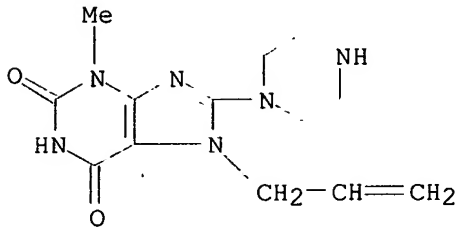
L5 ANSWER 100 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313255-35-5 REGISTRY
CN 1H-Purine-2,6-dione, 7-butyl-3,7-dihydro-3-methyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H22 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS

Searched by: Mary Hale 308-4258 CM-1 12D16



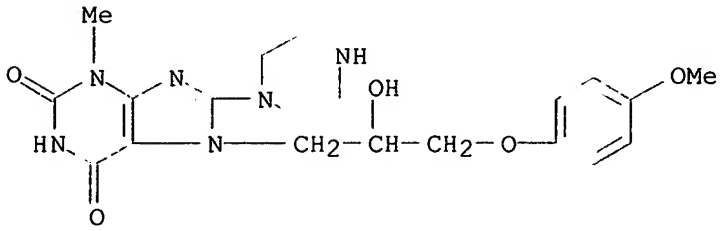
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 101 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 313230-36-3 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-8-(1-piperazinyl)-7-(2-propenyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H18 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

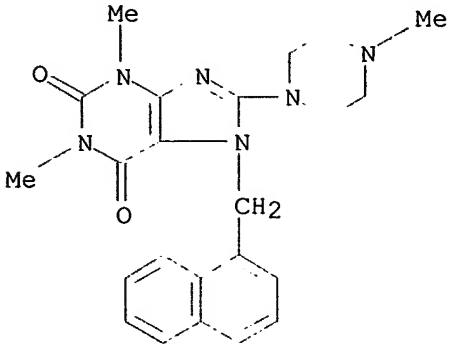
L5 ANSWER 102 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 312915-48-3 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-3-(4-methoxyphenoxy)propyl]-3-methyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H26 N6 O5
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

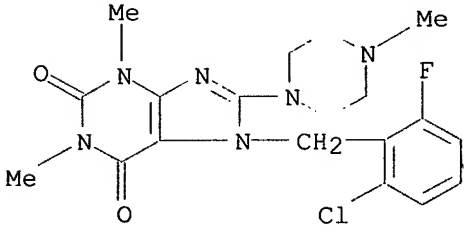
Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 103 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 309938-17-8 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)-7-(1-naphthalenylmethyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H26 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

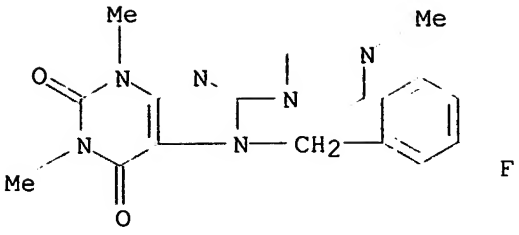
L5 ANSWER 104 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 309937-99-3 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(2-chloro-6-fluorophenyl)methyl]-3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
MF C19 H22 Cl F N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

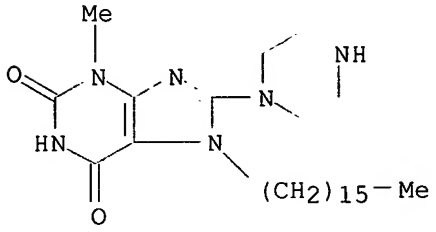
L5 ANSWER 105 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 309937-43-7 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(3-fluorophenyl)methyl]-3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H23 F N6 O2
SR Chemical Library
LC STN Files: CHEMCATS

Searched by: Mary Hale 308-4258 CM-1 12D16



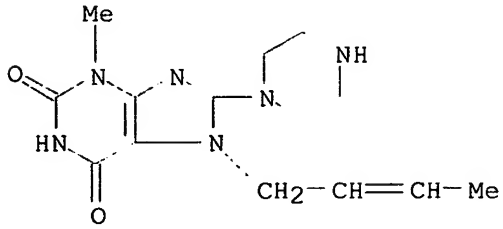
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 106 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 304876-71-9 REGISTRY
CN 1H-Purine-2,6-dione, 7-hexadecyl-3,7-dihydro-3-methyl-8-(1-piperazinyl)-
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C26 H46 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

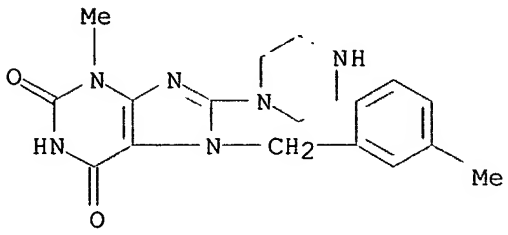
L5 ANSWER 107 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 303973-85-5 REGISTRY
CN 1H-Purine-2,6-dione, 7-(2-butenyl)-3,7-dihydro-3-methyl-8-(1-piperazinyl)-
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H20 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

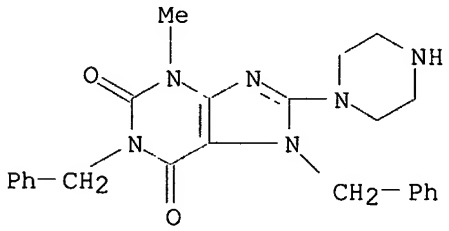
Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 108 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 303973-23-1 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-[(3-methylphenyl)methyl]-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H22 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

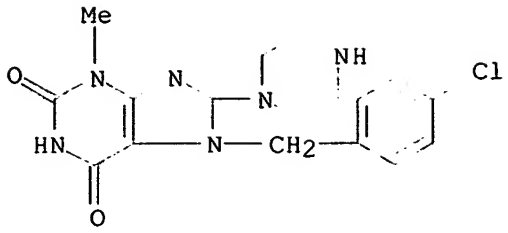
L5 ANSWER 109 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 303972-96-5 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-1,7-bis(phenylmethyl)-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H26 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 110 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 303971-30-4 REGISTRY
CN 1H-Purine-2,6-dione, 7-[(4-chlorophenyl)methyl]-3,7-dihydro-3-methyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H19 Cl N6 O2
SR Chemical Library
LC STN Files: CHEMCATS

Searched by: Mary Hale 308-4258 CM-1 12D16

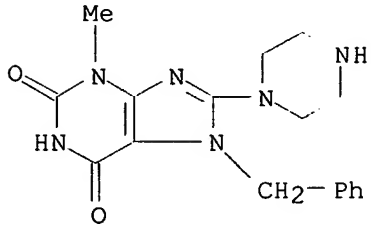


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 111 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 302942-21-8 REGISTRY
CN 7H-Purine-7-acetic acid, 8-bromo-1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-, compd. with 3,7-dihydro-3-methyl-7-(phenylmethyl)-8-(1-piperazinyl)-1H-purine-2,6-dione (1:1) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-(phenylmethyl)-8-(1-piperazinyl)-, mono(8-bromo-1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-7H-purine-7-acetate) (9CI)
MF C17 H20 N6 O2 . C8 H7 Br N4 O4
SR Chemical Library
LC STN Files: CHEMCATS

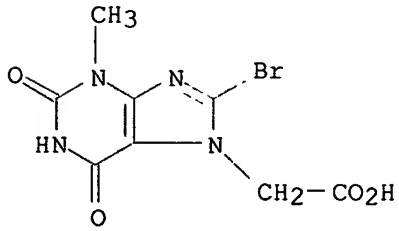
CM 1

CRN 299419-33-3
CMF C17 H20 N6 O2



CM 2

CRN 107608-69-5
CMF C8 H7 Br N4 O4

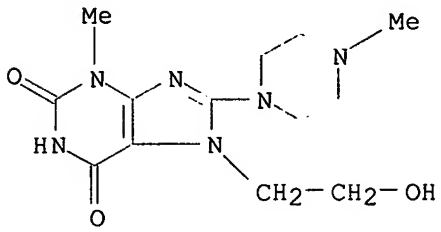


Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 112 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 302903-96-4 REGISTRY
CN Benzoic acid, 4-hydroxy-3-methoxy-, compd. with 3,7-dihydro-7-(2-hydroxyethyl)-3-methyl-8-(4-methyl-1-piperazinyl)-1H-purine-2,6-dione (1:1) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-(2-hydroxyethyl)-3-methyl-8-(4-methyl-1-piperazinyl)-, mono(4-hydroxy-3-methoxybenzoate) (salt) (9CI)
MF C13 H20 N6 O3 . C8 H8 O4
SR Chemical Library
LC STN Files: CHEMCATS

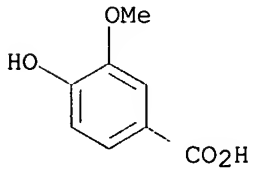
CM 1

CRN 302903-95-3
CMF C13 H20 N6 O3



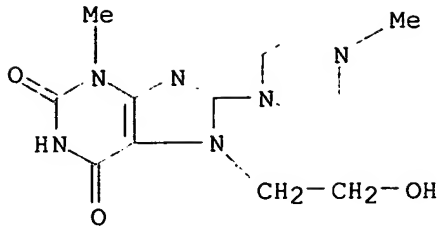
CM 2

CRN 121-34-6
CMF C8 H8 O4



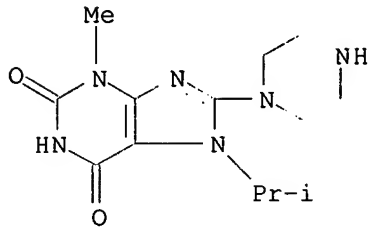
L5 ANSWER 113 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 302903-95-3 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-(2-hydroxyethyl)-3-methyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H20 N6 O3
CI COM
SR Chemical Library
LC STN Files: CHEMCATS

Searched by: Mary Hale 308-4258 CM-1 12D16



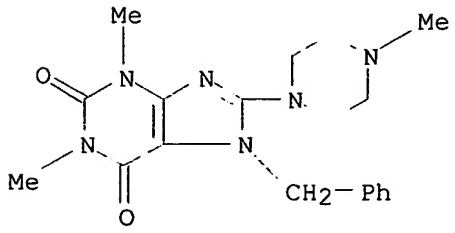
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 114 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 302800-67-5 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-(1-methylethyl)-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H20 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 115 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 302785-79-1 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H24 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



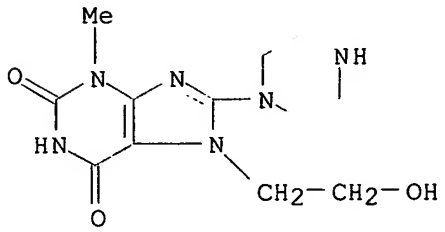
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 116 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 302778-39-8 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-(2-hydroxyethyl)-3-methyl-8-(1-piperazinyl)-, (2E)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C12 H18 N6 O3 . C4 H4 O4
SR Chemical Library
LC STN Files: CHEMCATS

CM 1

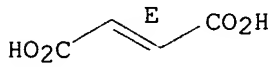
CRN 302777-00-0
CMF C12 H18 N6 O3



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

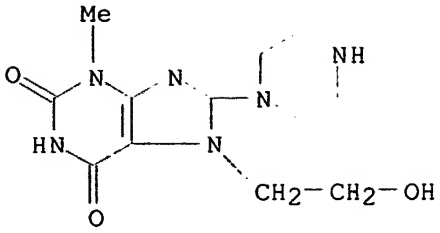


L5 ANSWER 117 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 302777-12-4 REGISTRY
CN Benzoic acid, 2-hydroxy-, compd. with 3,7-dihydro-7-(2-hydroxyethyl)-3-methyl-8-(1-piperazinyl)-1H-purine-2,6-dione (1:1) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-(2-hydroxyethyl)-3-methyl-8-(1-piperazinyl)-, mono(2-hydroxybenzoate) (salt) (9CI)
MF C12 H18 N6 O3 . C7 H6 O3
SR Chemical Library
LC STN Files: CHEMCATS

CM 1

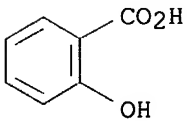
CRN 302777-00-0
CMF C12 H18 N6 O3

Searched by: Mary Hale 308-4258 CM-1 12D16



CM 2

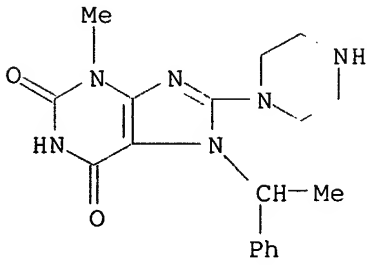
CRN 69-72-7
CMF C7 H6 O3



L5 ANSWER 118 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 302777-11-3 REGISTRY
CN Butanedioic acid, hydroxy-, compd. with 3,7-dihydro-3-methyl-7-(1-phenylethyl)-8-(1-piperazinyl)-1H-purine-2,6-dione (1:1) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-(1-phenylethyl)-8-(1-piperazinyl)-, hydroxybutanedioate (1:1) (9CI)
MF C18 H22 N6 O2 . C4 H6 O5
SR Chemical Library
LC STN Files: CHEMCATS

CM 1

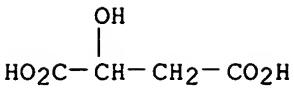
CRN 302777-10-2
CMF C18 H22 N6 O2



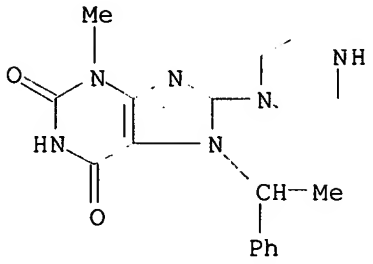
CM 2

CRN 6915-15-7
CMF C4 H6 O5

Searched by: Mary Hale 308-4258 CM-1 12D16



L5 ANSWER 119 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 302777-10-2 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-(1-phenylethyl)-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H22 N6 O2
CI COM
SR Chemical Library
LC STN Files: CHEMCATS

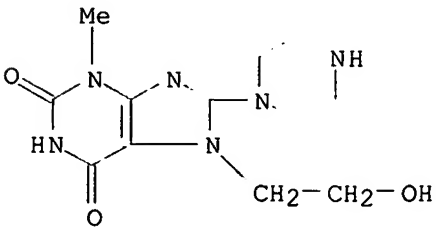


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 120 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 302777-01-1 REGISTRY
CN 1H-1,2,4-Triazole-3-carboxylic acid, 5-amino-, compd. with 3,7-dihydro-7-(2-hydroxyethyl)-3-methyl-8-(1-piperazinyl)-1H-purine-2,6-dione (1:1) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-(2-hydroxyethyl)-3-methyl-8-(1-piperazinyl)-, 5-amino-1H-1,2,4-triazole-3-carboxylate (1:1) (salt) (9CI)
MF C12 H18 N6 O3 . C3 H4 N4 O2
SR Chemical Library
LC STN Files: CHEMCATS

CM 1

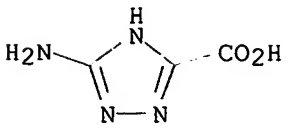
CRN 302777-00-0
CMF C12 H18 N6 O3



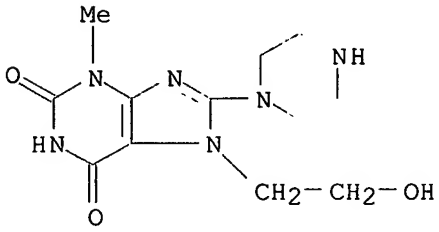
Searched by: Mary Hale 308-4258 CM-1 12D16

CM 2

CRN 3641-13-2
CMF C3 H4 N4 O2



L5 ANSWER 121 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 302777-00-0 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-(2-hydroxyethyl)-3-methyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H18 N6 O3
CI COM
SR Chemical Library



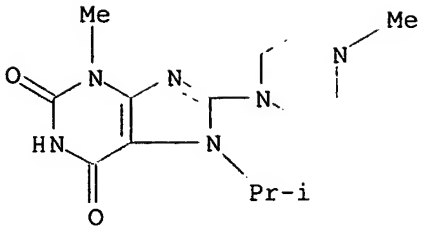
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 122 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 302590-35-8 REGISTRY
CN Butanedioic acid, hydroxy-, compd. with 3,7-dihydro-3-methyl-7-(1-methylethyl)-8-(4-methyl-1-piperazinyl)-1H-purine-2,6-dione (1:1) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-(1-methylethyl)-8-(4-methyl-1-piperazinyl)-, hydroxybutanedioate (1:1) (9CI)
MF C14 H22 N6 O2 . C4 H6 O5
SR Chemical Library
LC STN Files: CHEMCATS

CM 1

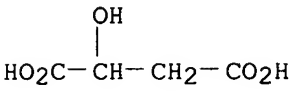
CRN 302590-34-7
CMF C14 H22 N6 O2

Searched by: Mary Hale 308-4258 CM-1 12D16

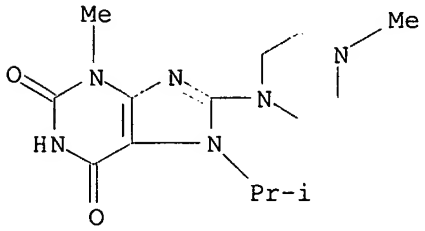


CM 2

CRN 6915-15-7
CMF C4 H6 O5



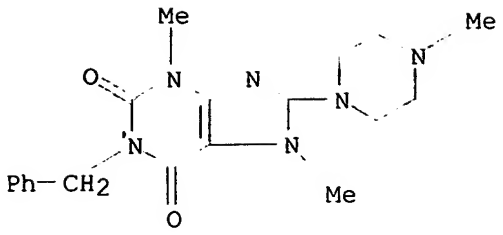
L5 ANSWER 123 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 302590-34-7 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-(1-methylethyl)-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H22 N6 O2
CI COM
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

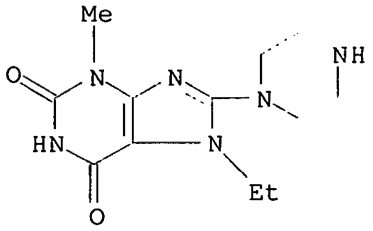
L5 ANSWER 124 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 300591-60-0 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl-8-(4-methyl-1-piperazinyl)-1-(phenylmethyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H24 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS

Searched by: Mary Hale 308-4258 CM-1 12D16



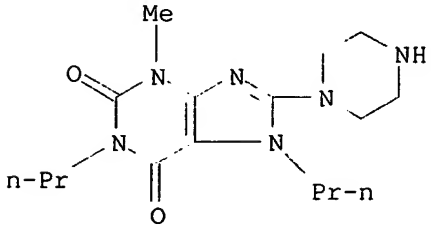
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 125 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 300391-56-4 REGISTRY
CN 1H-Purine-2,6-dione, 7-ethyl-3,7-dihydro-3-methyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H18 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

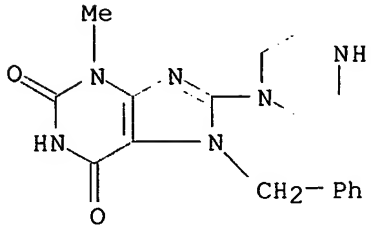
L5 ANSWER 126 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 299421-57-1 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-8-(1-piperazinyl)-1,7-dipropyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H26 N6 O2
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

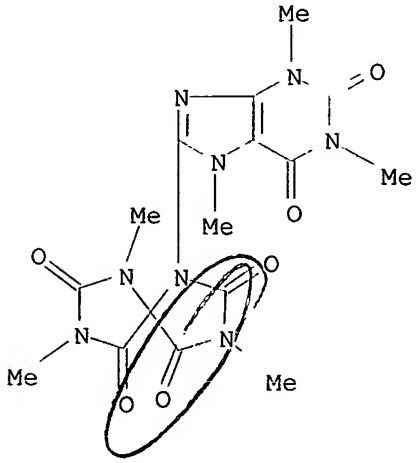
Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 127 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 299419-33-3 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3-methyl-7-(phenylmethyl)-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H20 N6 O2
CI COM
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 128 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 122776-37-8 REGISTRY
CN 1,3,6,8-Tetraazaspiro[4.4]nonane-2,4,7,9-tetrone, 1,3,8-trimethyl-6-(2,3,6,7-tetrahydro-1,3,7-trimethyl-2,6-dioxo-1H-purin-8-yl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H18 N8 O6
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

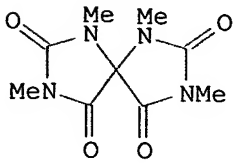
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 111:153495 Addition of electrophilic radicals to caffeine:

Searched by: Mary Hale 308-4258 CM-1 12D16

synthetic aspects and influence of the peroxidic initiators. Zylber, J.; Ouazzani-Chahdi, L.; Lefort, D.; Chiaroni, A.; Riche, C. (Lab. Electrochim. Catal. Synth. Org., CNRS, Thiais, 94320, Fr.). Tetrahedron, 45(3), 721-32 (English) 1989. CODEN: TETRAB. ISSN: 0040-4020.

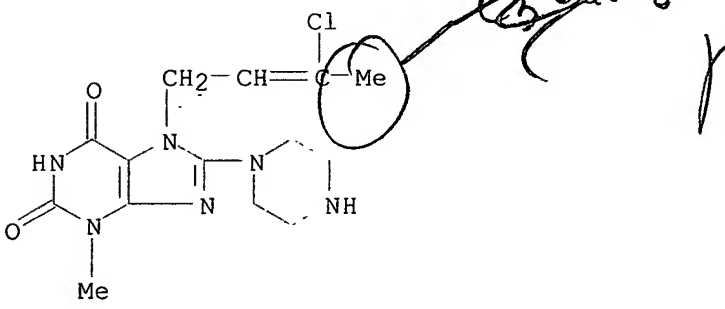
GI



I

AB Electrophilic radicals, such as .bul.CHRCO2Me(R = H, Me, CO2Me) and .bul.CCl3 radical were added directly at C-8 of, the model purine compd., caffeine to give 8-substituted derivs. in fairly good yields. The unexpected reaction of caffeine with oxy radicals from the initiators (BzO.bul., Me3COO.bul.) gave C-5 substituted 1,3,7-trimethyl-5,7-dihydrouric acid derivs. and spirodihydantoin adduct I, whose crystal structure is reported.

L5 ANSWER 129 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 106939-29-1 REGISTRY
CN 1H-Purine-2,6-dione, 7-(3-chloro-2-butenyl)-3,7-dihydro-3-methyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H19 Cl N6 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS, TOXCENTER, TOXLIT



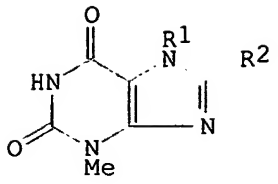
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 106:95577 Synthesis and biological activity of 3-methyl, 7- or 8-alkyl-, 7,8-dialkyl, heterocyclic, and cyclohexylaminoxanthines. Romanenko, N. I.; Fedulova, I. V.; Primenko, B. O.; Orestenko, L. P. (Zaporozh. Med. Inst., Zaporozhe, USSR). Farm. Zh. (Kiev) (5), 41-4 (Ukranian) 1986. CODEN: FRZKAP. ISSN: 0367-3057.

GI

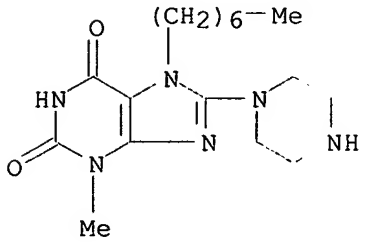
Searched by: Mary Hale 308-4258 CM-1 12D16



I

AB Seventeen title compds. (I; R1 = heptyl, nonyl, or CH2CH:C(Cl)Me; R2 = NMe2, NEt2, piperidino, cyclohexylamino, NHCH2Ph, piperazino, morpholino, NHNH2, N(CH2CH2OH)2, etc.) were prepd. by reacting the K salt of 8-bromo-3-methylxanthine with appropriate alkyl halides followed by condensation with appropriate primary or secondary amines. Toxicity studies in mice showed I to be less toxic than aminazine. Most I exhibited diuretic activity in rats, and some exhibited analeptic activity as well. Many I exhibited antimicrobial activity in vitro against both bacteria and fungi. The most active diuretics contained morpholino, piperidino, or N-benzyl groups at the 8-position.

L5 ANSWER 130 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 106939-21-3 REGISTRY
CN 1H-Purine-2,6-dione, 7-heptyl-3,7-dihydro-3-methyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H28 N6 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS, TOXCENTER, TOXLIT



NO provided

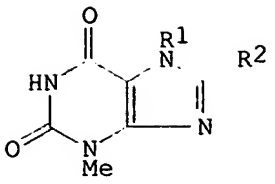
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 106:95577 Synthesis and biological activity of 3-methyl, 7- or 8-alkyl-, 7,8-dialkyl, heterocyclic, and cyclohexylaminoxanthines. Romanenko, N. I.; Fedulova, I. V.; Primenko, B. O.; Orestenko, L. P. (Zaporozh. Med. Inst., Zaporozhe, USSR). Farm. Zh. (Kiev) (5), 41-4 (Ukranian) 1986. CODEN: FRZKAP. ISSN: 0367-3057.

GI

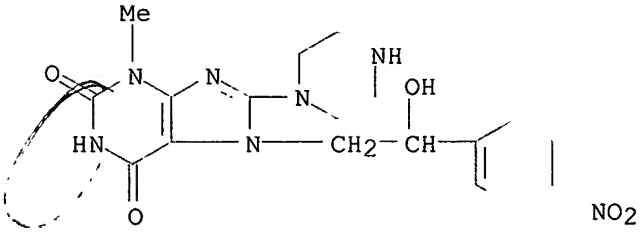
Searched by: Mary Hale 308-4258 CM-1 12D16



I

AB Seventeen title compds. (I; R1 = heptyl, nonyl, or CH2CH:C(Cl)Me; R2 = NMe2, NEt2, piperidino, cyclohexylamino, NHCH2Ph, piperazino, morpholino, NHNH2, N(CH2CH2OH)2, etc.) were prepd. by reacting the K salt of 8-bromo-3-methylxanthine with appropriate alkyl halides followed by condensation with appropriate primary or secondary amines. Toxicity studies in mice showed I to be less toxic than aminazine. Most I exhibited diuretic activity in rats, and some exhibited analeptic activity as well. Many I exhibited antimicrobial activity in vitro against both bacteria and fungi. The most active diuretics contained morpholino, piperidino, or N-benzyl groups at the 8-position.

L5 ANSWER 131 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 105522-62-1 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-2-(4-nitrophenyl)ethyl]-3-methyl-8-(1-piperazinyl)-, monohydrochloride (9CI) (CA INDEX NAME)
MF C18 H21 N7 O5 . Cl H
SR CA
LC STN Files: CA, CAPLUS, RTECS*
(*File contains numerically searchable property data)
CRN (105522-61-0)



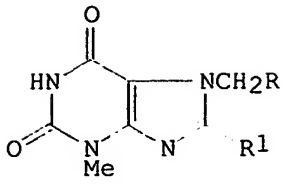
● HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 105:226150 Synthesis, neurotropic and diuretic activity of 7,8-disubstituted 3-methylxanthines. Samura, B. A.; Fedulova, I. V.; Romanenko, B. A.; Priimenko, B. A.; Chervinskii, A. Yu.; Garmash, S. N.; Troshin, D. A. (Zaporozh. Med. Inst., Zaporozh, USSR). Khim.-Farm. Zh., 20(1), 52-5 (Russian) 1986. CODEN: KHFZAN. ISSN: 0023-1134.

GI

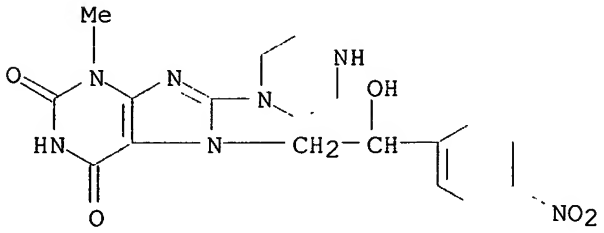
Searched by: Mary Hale 308-4258 CM-1 12D16



I

AB The title compds. I (R = Ph, CH2OPh, CH(OH)C6H4NO2-p, R1 = 2-furylmethylamino, morpholino, hexamethylenimino, NHCH2CH2OH, NEt2, piperazino, SCH2CO2H), useful as psychotropics and diuretics, were prepd. in 24-94% yields from I (R1 = Br) by amination with appropriate amines or by reaction with HSCH2CO2H. The hydrochloride of I [R = CH(OH)C6H4NO2-p, R1 = piperazino] increased urinary flow 180.7% compared to a control and potentiated narcotic sleep 147.0% compared to a control.

L5 ANSWER 132 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 105522-61-0 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-2-(4-nitrophenyl)ethyl]-3-methyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H21 N7 O5
CI COM
SR CA
LC STN Files: CA, CAPLUS, CASREACT

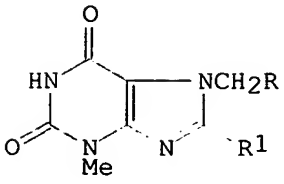


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 105:226150 Synthesis, neurotropic and diuretic activity of 7,8-disubstituted 3-methylxanthines. Samura, B. A.; Fedulova, I. V.; Romanenko, B. A.; Priimenko, B. A.; Chervinskii, A. Yu.; Garmash, S. N.; Troshin, D. A. (Zaporozh. Med. Inst., Zaporozh, USSR). Khim.-Farm. Zh., 20(1), 52-5 (Russian) 1986. CODEN: KHFZAN. ISSN: 0023-1134.

GI

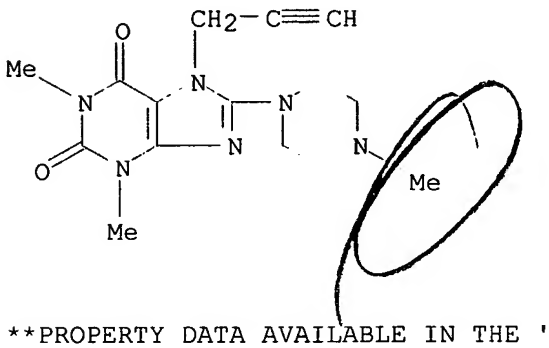


I

Searched by: Mary Hale 308-4258 CM-1 12D16

AB The title compds. I (R = Ph, CH2OPh, CH(OH)C6H4NO2-p, R1 = 2-furylmethylamino, morpholino, hexamethylenimino, NHCH2CH2OH, NEt2, piperazino, SCH2CO2H), useful as psychotropics and diuretics, were prepd. in 24-94% yields from I (R1 = Br) by amination with appropriate amines or by reaction with HSCH2CO2H. The hydrochloride of I [R = CH(OH)C6H4NO2-p, R1 = piperazino] increased urinary flow 180.7% compared to a control and potentiated narcotic sleep 147.0% compared to a control.

L5 ANSWER 133 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 97725-83-2 REGISTRY
CN Theophylline, 8-(4-methyl-1-piperazinyl)-7-(2-propynyl)- (7CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H20 N6 O2
SR CAOLD
LC STN Files: BEILSTEIN*, CAOLD
(*File contains numerically searchable property data)

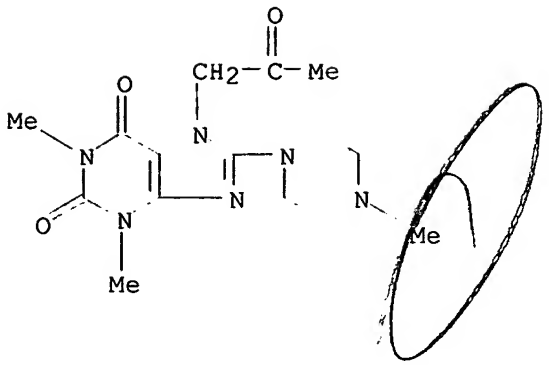


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L5 ANSWER 134 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 97490-51-2 REGISTRY
CN Theophylline, 7-acetonyl-8-(4-methyl-1-piperazinyl)-, hydrochloride (7CI) (CA INDEX NAME)
MF C15 H22 N6 O3 . x Cl H
SR CAOLD
LC STN Files: CAOLD
CRN (743-53-3)

Searched by: Mary Hale 308-4258 CM-1 12D16



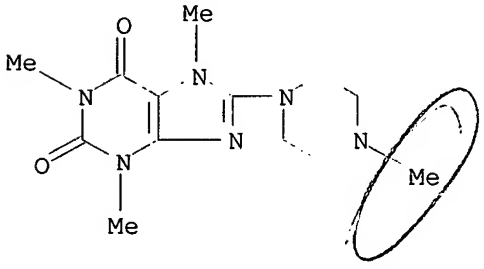
●x HCl

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L5 ANSWER 135 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 96987-48-3 REGISTRY
CN Caffeine, 8-(4-methyl-1-piperazinyl)-, methobromide (7CI) (CA INDEX NAME)
MF C13 H20 N6 O2 . C H3 Br
LC STN Files: CAOLD

CM 1

CRN 96294-94-9
CMF C13 H20 N6 O2



CM 2

CRN 74-83-9
CMF C H3 Br

Br—CH_3

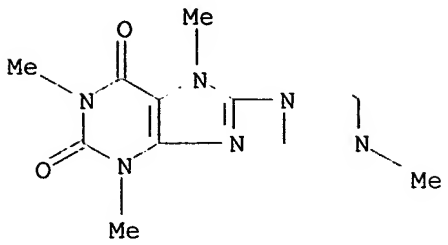
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L5 ANSWER 136 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 96986-88-8 REGISTRY
CN Caffeine, 8-(4-methyl-1-piperazinyl)-, methiodide (7CI) (CA INDEX NAME)
MF C13 H20 N6 O2 . C H3 I
LC STN Files: CAOLD

CM 1

Searched by: Mary Hale 308-4258 CM-1 12D16

CRN 96294-94-9
CMF C13 H20 N6 O2



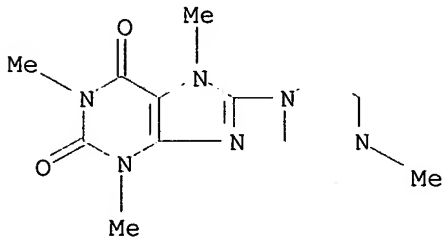
CM 2

CRN 74-88-4
CMF C H3 I

H_3C-I

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L5 ANSWER 137 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 96294-95-0 REGISTRY
CN Caffeine, 8-(4-methyl-1-piperazinyl)-, hydrochloride (6CI, 7CI) (CA INDEX NAME)
MF C13 H20 N6 O2 . x Cl H
LC STN Files: BEILSTEIN*, CAOLD
(*File contains numerically searchable property data)
CRN (96294-94-9)



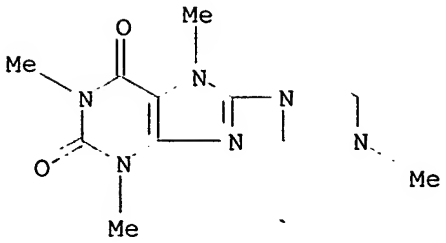
●x HCl

2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L5 ANSWER 138 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 96294-94-9 REGISTRY
CN Caffeine, 8-(4-methyl-1-piperazinyl)- (7CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H20 N6 O2
CI COM
LC STN Files: BEILSTEIN*, CAOLD, CHEMCATS

Searched by: Mary Hale 308-4258 CM-1 12D16

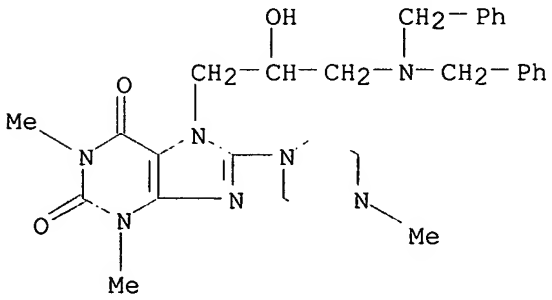
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L5 ANSWER 139 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 87080-34-0 REGISTRY
CN 1H-Purine-2,6-dione, 7-[3-[bis(phenylmethyl)amino]-2-hydroxypropyl]-3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C29 H37 N7 O3
LC STN Files: CA, CAPLUS

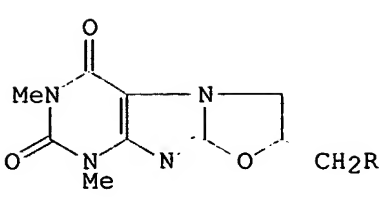


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 99:139617 Synthesis and properties of 7- and 8-piperazinyl derivatives of theophylline. Gorczyca, Maria; Pawlowski, Maciej; Lucka-Sobstel, Barbara (Dep. Pharm. Chem., Sch. Med., Krakow, 31-065, Pol.). Acta Pol. Pharm., 39(5-6), 315-21 (Polish) 1982. CODEN: APPHAX. ISSN: 0001-6837.
GI

Searched by: Mary Hale 308-4258 CM-1 12D16



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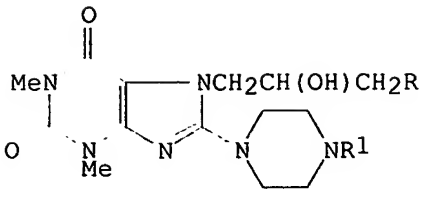

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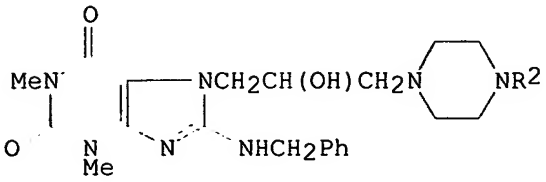
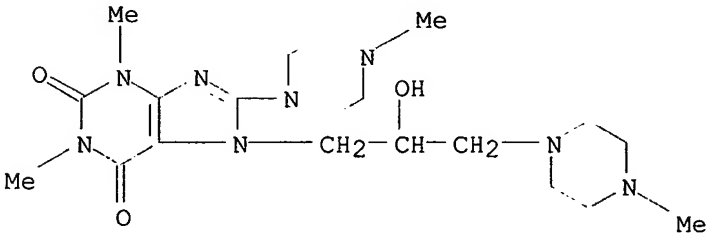


III

AB Aminolysis of the oxazole ring in I (R = H, Cl) with an N-substituted piperazine yielded II (R = H, Cl; R1 = Me, CH2CH2OH). II (R = Cl) were treated with an amine in the presence of KOH to give II (R = PhCH2NH, R1 = Me, CH2CH2OH; R = 4-methyl-1-piperazinyl, R1 = Me). An analogous reaction of I (R = Cl) with PhCH2NH2 followed by reaction with an N-substituted piperazine gave III (R2 = CH2CH2OH, CO2Et, Ph). II and III are potential cardiovascular agents.

L5 ANSWER 140 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 87080-33-9 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-[2-hydroxy-3-(4-methyl-1-piperazinyl)propyl]-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H34 N8 O3
LC STN Files: CA, CAPLUS



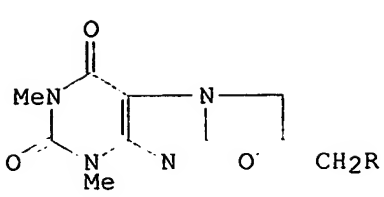
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

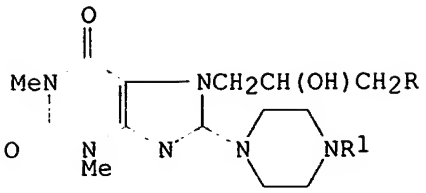
REFERENCE 1: 99:139617 Synthesis and properties of 7- and 8-piperazinyl derivatives of theophylline. Gorczyca, Maria; Pawlowski, Maciej; Lucka-Sobstel, Barbara (Dep. Pharm. Chem., Sch. Med., Krakow, 31-065, Pol.). Acta Pol. Pharm., 39(5-6), 315-21 (Polish) 1982. CODEN: APPHAX. ISSN: 0001-6837.

GI

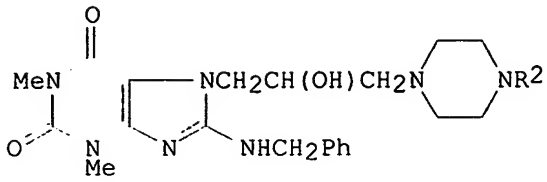
Searched by: Mary Hale 308-4258 CM-1 12D16



I



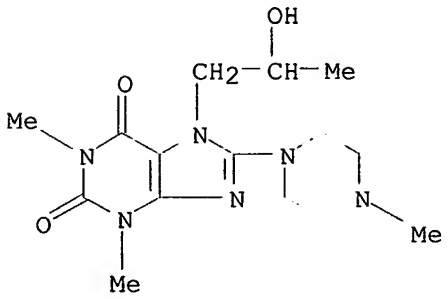
II



III

AB Aminolysis of the oxazole ring in I (R = H, Cl) with an N-substituted piperazine yielded II (R = H, Cl; R1 = Me, CH2CH2OH). II (R = Cl) were treated with an amine in the presence of KOH to give II (R = PhCH2NH, R1 = Me, CH2CH2OH; R = 4-methyl-1-piperazinyl, R1 = Me). An analogous reaction of I (R = Cl) with PhCH2NH2 followed by reaction with an N-substituted piperazine gave III (R2 = CH2CH2OH, CO2Et, Ph). II and III are potential cardiovascular agents.

L5 ANSWER 141 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 87080-32-8 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-7-(2-hydroxypropyl)-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H24 N6 O3
LC STN Files: CA, CAPLUS



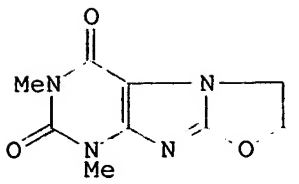
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

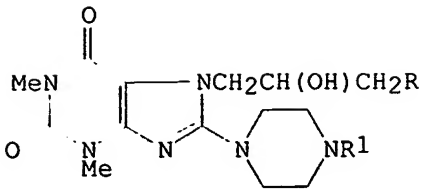
REFERENCE 1: 99:139617 Synthesis and properties of 7- and 8-piperazinyl derivatives of theophylline. Gorczyca, Maria; Pawlowski, Maciej; Lucka-Sobstel, Barbara (Dep. Pharm. Chem., Sch. Med., Krakow, 31-065, Pol.). Acta Pol. Pharm., 39(5-6), 315-21 (Polish) 1982. CODEN: APPHAX. ISSN: 0001-6837.

GI

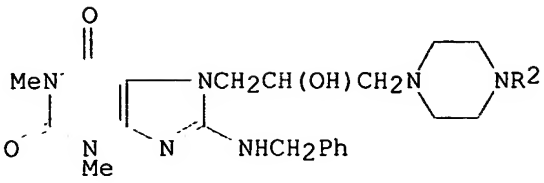
Searched by: Mary Hale 308-4258 CM-1 12D16



I



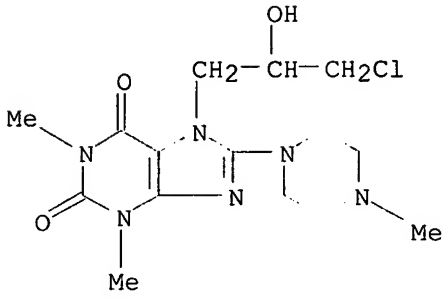
II



III

AB Aminolysis of the oxazole ring in I (R = H, Cl) with an N-substituted piperazine yielded II (R = H, Cl; R1 = Me, CH2CH2OH). II (R = Cl) were treated with an amine in the presence of KOH to give II (R = PhCH2NH, R1 = Me, CH2CH2OH; R = 4-methyl-1-piperazinyl, R1 = Me). An analogous reaction of I (R = Cl) with PhCH2NH2 followed by reaction with an N-substituted piperazine gave III (R2 = CH2CH2OH, CO2Et, Ph). II and III are potential cardiovascular agents.

L5 ANSWER 142 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 87080-28-2 REGISTRY
CN 1H-Purine-2,6-dione, 7-(3-chloro-2-hydroxypropyl)-3,7-dihydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H23 Cl N6 O3
LC STN Files: CA, CAPLUS



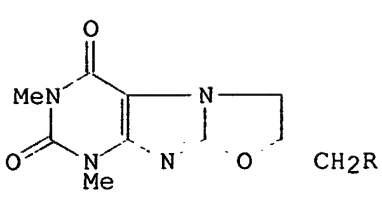
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 99:139617 Synthesis and properties of 7- and 8-piperazinyl derivatives of theophylline. Gorczyca, Maria; Pawlowski, Maciej; Lucka-Sobstel, Barbara (Dep. Pharm. Chem., Sch. Med., Krakow, 31-065, Pol.). Acta Pol. Pharm., 39(5-6), 315-21 (Polish) 1982. CODEN: APPHAX. ISSN: 0001-6837.

GI

Searched by: Mary Hale 308-4258 CM-1 12D16



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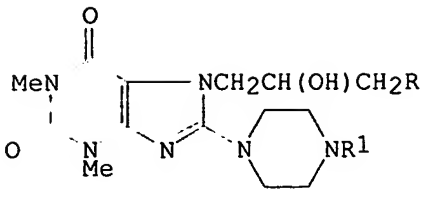
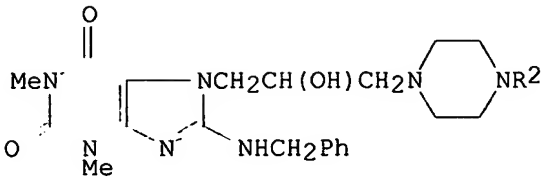


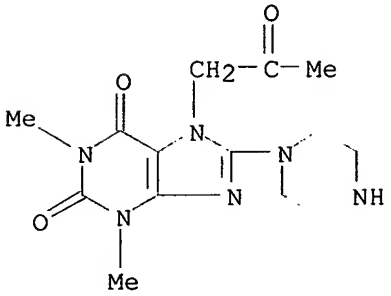
II



III

AB Aminolysis of the oxazole ring in I (R = H, Cl) with an N-substituted piperazine yielded II (R = H, Cl; R1 = Me, CH2CH2OH). II (R = Cl) were treated with an amine in the presence of KOH to give II (R = PhCH2NH, R1 = Me, CH2CH2OH; R = 4-methyl-1-piperazinyl, R1 = Me). An analogous reaction of I (R = Cl) with PhCH2NH2 followed by reaction with an N-substituted piperazine gave III (R2 = CH2CH2OH, CO2Et, Ph). II and III are potential cardiovascular agents.

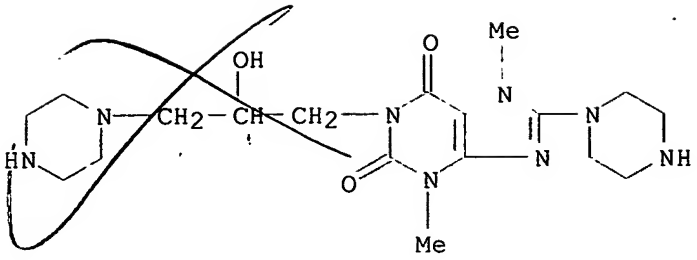
L5 ANSWER 143 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 74039-61-5 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-7-(2-oxopropyl)-8-(1-piperazinyl)-, hydrochloride (9CI) (CA INDEX NAME)
MF C14 H20 N6 O3 . x Cl H
LC STN Files: RTECS*
(*File contains numerically searchable property data)
CRN (24961-80-6)



● x HCl

L5 ANSWER 144 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 69408-23-7 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1-[2-hydroxy-3-(1-piperazinyl)propyl]-3,7-dimethyl-8-(1-piperazinyl)-, trihydrochloride (9CI) (CA INDEX NAME)
MF C18 H30 N8 O3 . 3 Cl H
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Searched by: Mary Hale 308-4258 CM-1 12D16

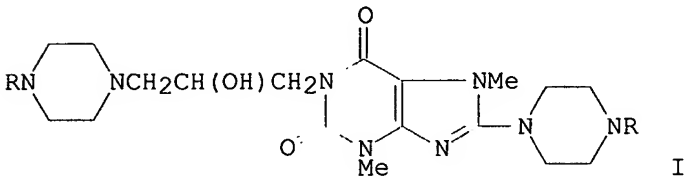


● 3 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 90:103924 Piperazine derivatives of dimethylxanthines. VI. Reactions of 1-(2,3-epoxy)propyl-8-bromotheobromine with piperazines. Zejc, Alfred; Kiec-Kononowicz, Katarzyna; Pawlowski, Maciej (Sch. Med., Dep. Pharm. Chem., Krakow, Pol.). Acta Pol. Pharm., 35(4), 417-21 (Polish) 1978. CODEN: APPHAX. ISSN: 0001-6837.

GI



I

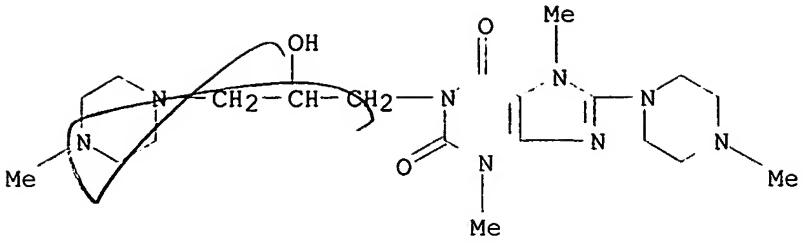
AB The title deriv. of theobromine refluxed in PrOH with N-aryl and N-alkyl derivs. of piperazine gave I (R = Ph, PhCH2, 4-ClC6H4, 4-MeC6H4, Me, HOCH2CH2, EtO2C (II)]. On heating with concd. HCl, II underwent hydrolysis and decarboxylation to yield I (R = H). All yields were almost quant; I were synthesized as potential diuretics, spasmolytics, antihistaminics, and cardiostimulants.

L5 ANSWER 145 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 69408-16-8 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1-[2-hydroxy-3-(4-methyl-1-piperazinyl)propyl]-3,7-dimethyl-8-(4-methyl-1-piperazinyl)-, ethanedioate (1:3) (salt) (9CI) (CA INDEX NAME)
MF C20 H34 N8 O3 . 3 C2 H2 O4
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

CM 1

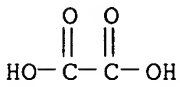
CRN 69408-15-7
CMF C20 H34 N8 O3

Searched by: Mary Hale 308-4258 CM-1 12D16



CM 2

CRN 144-62-7
CMF C2 H2 O4



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 90:103924 Piperazine derivatives of dimethylxanthines. VI. Reactions of 1-(2,3-epoxy)propyl-8-bromotheobromine with piperazines. Zejc, Alfred; Kiec-Kononowicz, Katarzyna; Pawlowski, Maciej (Sch. Med., Dep. Pharm. Chem., Krakow, Pol.). Acta Pol. Pharm., 35(4), 417-21 (Polish) 1978. CODEN: APPHAX. ISSN: 0001-6837.

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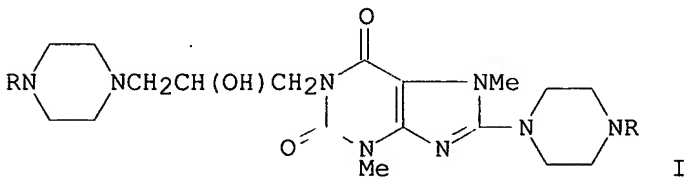
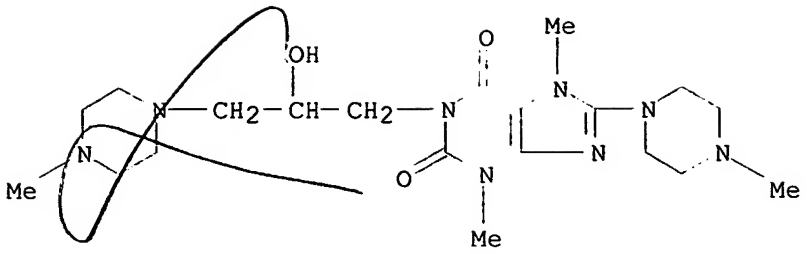


I

AB The title deriv. of theobromine refluxed in PrOH with N-aryl and N-alkyl derivs. of piperazine gave I (R = Ph, PhCH2, 4-ClC6H4, 4-MeC6H4, Me, HOCH2CH2, EtO2C (II)]. On heating with concd. HCl, II underwent hydrolysis and decarboxylation to yield I (R = H). All yields were almost quant; I were synthesized as potential diuretics, spasmolytics, antihistaminics, and cardiostimulants.

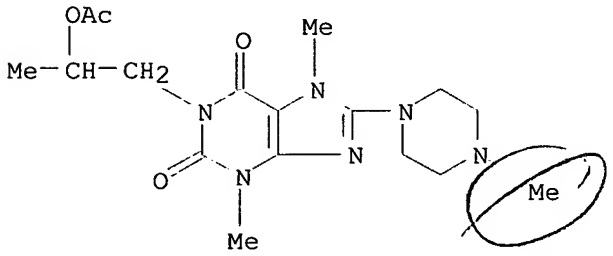
L5 ANSWER 146 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 69408-15-7 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1-[2-hydroxy-3-(4-methyl-1-piperazinyl)propyl]-3,7-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H34 N8 O3
CI COM
LC STN Files: BEILSTEIN*
(*File contains numerically searchable property data)

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 147 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 67162-78-1 REGISTRY
CN 1H-Purine-2,6-dione, 1-[2-(acetyloxy)propyl]-3,7-dihydro-3,7-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H26 N6 O4
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:109376 Piperazine derivatives of dimethylxanthines. V. Preparation and properties of 8-piperazino- and 1-.beta.-hydroxypropyl-8-piperazinotheobromines. Cygankiewicz, Andrzej; Gorczyca, Maria; Zejc, Alfred; Zimon, Romuald (Dep. Pharm. Chem., Sch. Med., Krakow, Pol.). Acta Pol. Pharm., 34(6), 607-12 (Polish) 1977. CODEN: APPHAX. ISSN: 0001-6837.

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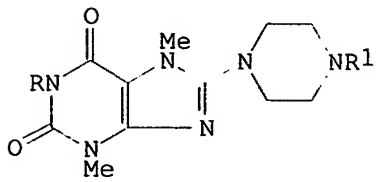
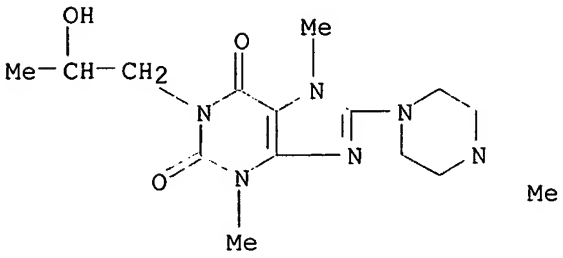


I, R=H
II, R=$CH_2CH(OH)Me$

Searched by: Mary Hale 308-4258 CM-1 12D16

AB 8-Bromotheobromine and anhyd. piperazine heated in MeOCH2CH2OH gave 67% I (R1 = H). I [R1 = Me, CH2CH2OH, and CH2CH(OH)Me] were prepd. analogously in 68-72% yields. I heated in PrOH with 2,3-epoxypropane in presence of pyridine gave 48-75% II [R1 = H, Me, CH2CH(OH)Me], which were also obtained in the reaction of 1-(.beta.-hydroxypropyl)-8-bromotheobromine with the appropriately substituted piperazine. All I and II were characterized as HCl or HBr salts, and most of the hydroxylated I and II, also as the Ac derivs. I and II were synthesized as potential spasmolytics and antihistaminics.

L5 ANSWER 148 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 67162-77-0 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1-(2-hydroxypropyl)-3,7-dimethyl-8-(4-methyl-1-piperazinyl)-, monohydrobromide (9CI) (CA INDEX NAME)
MF C15 H24 N6 O3 . Br H
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)
CRN (67162-76-9)



● HBr

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:109376 Piperazine derivatives of dimethylxanthines. V. Preparation and properties of 8-piperazino- and 1-.beta.-hydroxypropyl-8-piperazinotheobromines. Cygankiewicz, Andrzej; Gorczyca, Maria; Zejc, Alfred; Zimon, Romuald (Dep. Pharm. Chem., Sch. Med., Krakow, Pol.). Acta Pol. Pharm., 34(6), 607-12 (Polish) 1977. CODEN: APPHAX. ISSN: 0001-6837.

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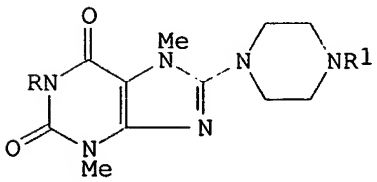

I, R=H
II, R=$CH_2CH(OH)Me$

AB 8-Bromotheobromine and anhyd. piperazine heated in MeOCH2CH2OH gave 67% I (R1 = H). I [R1 = Me, CH2CH2OH, and CH2CH(OH)Me] were prepd. analogously in 68-72% yields. I heated in PrOH with 2,3-epoxypropane in presence of pyridine gave 48-75% II [R1 = H, Me, CH2CH(OH)Me], which were also

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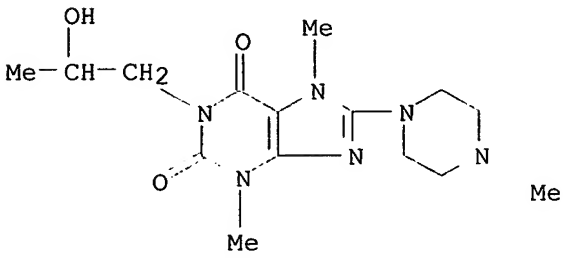
obtained in the reaction of 1-(.beta.-hydroxypropyl)-8-bromotheobromine with the appropriately substituted piperazine. All I and II were characterized as HCl or HBr salts, and most of the hydroxylated I and II, also as the Ac derivs. I and II were synthesized as potential spasmolytics and antihistaminics.

L5 ANSWER 149 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 67162-76-9 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1-(2-hydroxypropyl)-3,7-dimethyl-8-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H24 N6 O3
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:109376 Piperazine derivatives of dimethylxanthines. V. Preparation and properties of 8-piperazino- and 1-.beta.-hydroxypropyl-8-piperazinotheobromines. Cygankiewicz, Andrzej; Gorczyca, Maria; Zejc, Alfred; Zimon, Romuald (Dep. Pharm. Chem., Sch. Med., Krakow, Pol.). Acta Pol. Pharm., 34(6), 607-12 (Polish) 1977. CODEN: APPHAX. ISSN: 0001-6837.

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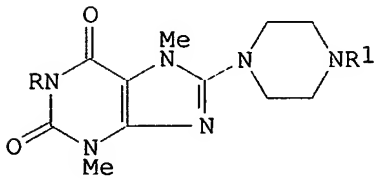
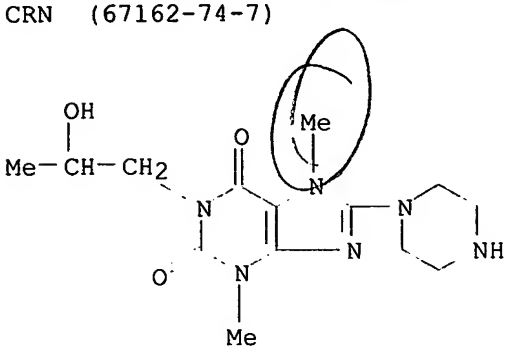


I, R=H
II, R=$CH_2CH(OH)Me$

AB 8-Bromotheobromine and anhyd. piperazine heated in MeOCH2CH2OH gave 67% I (R1 = H). I [R1 = Me, CH2CH2OH, and CH2CH(OH)Me] were prepd. analogously in 68-72% yields. I heated in PrOH with 2,3-epoxypropane in presence of pyridine gave 48-75% II [R1 = H, Me, CH2CH(OH)Me], which were also obtained in the reaction of 1-(.beta.-hydroxypropyl)-8-bromotheobromine with the appropriately substituted piperazine. All I and II were characterized as HCl or HBr salts, and most of the hydroxylated I and II, also as the Ac derivs. I and II were synthesized as potential spasmolytics and antihistaminics.

Searched by: Mary Hale 308-4258 CM-1 12D16

L5 ANSWER 150 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 67162-75-8 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1-(2-hydroxypropyl)-3,7-dimethyl-8-(1-piperazinyl)-, dihydrobromide (9CI) (CA INDEX NAME)
MF C14 H22 N6 O3 . 2 Br H
LC STN Files: CA, CAPLUS
CRN (67162-74-7)



●2 HBr

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:109376 Piperazine derivatives of dimethylxanthines. V. Preparation and properties of 8-piperazino- and 1-.beta.-hydroxypropyl-8-piperazinotheobromines. Cygankiewicz, Andrzej; Gorczyca, Maria; Zejc, Alfred; Zimon, Romuald (Dep. Pharm. Chem., Sch. Med., Krakow, Pol.). Acta Pol. Pharm., 34(6), 607-12 (Polish) 1977. CODEN: APPHAX. ISSN: 0001-6837.

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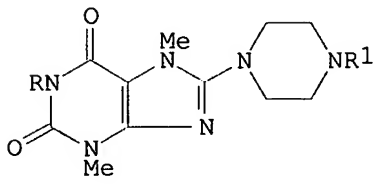


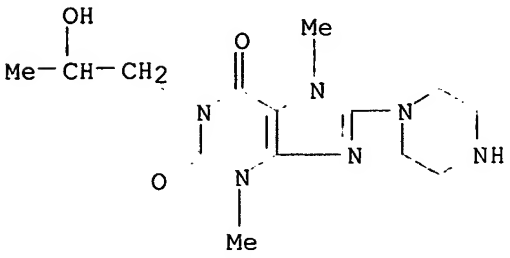
I, R=H
II, R=$CH_2CH(OH)Me$

AB 8-Bromotheobromine and anhyd. piperazine heated in MeOCH2CH2OH gave 67% I (R1 = H). I [R1 = Me, CH2CH2OH, and CH2CH(OH)Me] were prepd. analogously in 68-72% yields. I heated in PrOH with 2,3-epoxypropane in presence of pyridine gave 48-75% II [R1 = H, Me, CH2CH(OH)Me], which were also obtained in the reaction of 1-(.beta.-hydroxypropyl)-8-bromotheobromine with the appropriately substituted piperazine. All I and II were characterized as HCl or HBr salts, and most of the hydroxylated I and II, also as the Ac derivs. I and II were synthesized as potential spasmolytics and antihistaminics.

L5 ANSWER 151 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 67162-74-7 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1-(2-hydroxypropyl)-3,7-dimethyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD

Searched by: Mary Hale 308-4258 CM-1 12D16

MF C14 H22 N6 O3
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

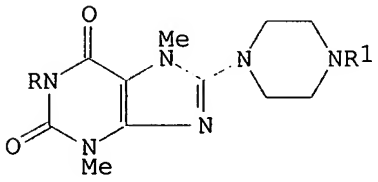


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:109376 Piperazine derivatives of dimethylxanthines. V. Preparation and properties of 8-piperazino- and 1-.beta.-hydroxypropyl-8-piperazinotheobromines. Cygankiewicz, Andrzej; Gorczyca, Maria; Zejc, Alfred; Zimon, Romuald (Dep. Pharm. Chem., Sch. Med., Krakow, Pol.). Acta Pol. Pharm., 34(6), 607-12 (Polish) 1977. CODEN: APPHAX. ISSN: 0001-6837.

GI

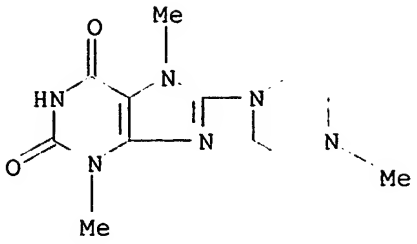


I, R=H
II, R=$CH_2CH(OH)Me$

AB 8-Bromotheobromine and anhyd. piperazine heated in MeOCH2CH2OH gave 67% I (R1 = H). I [R1 = Me, CH2CH2OH, and CH2CH(OH)Me] were prepd. analogously in 68-72% yields. I heated in PrOH with 2,3-epoxypropane in presence of pyridine gave 48-75% II [R1 = H, Me, CH2CH(OH)Me], which were also obtained in the reaction of 1-(.beta.-hydroxypropyl)-8-bromotheobromine with the appropriately substituted piperazine. All I and II were characterized as HCl or HBr salts, and most of the hydroxylated I and II, also as the Ac derivs. I and II were synthesized as potential spasmolytics and antihistaminics.

L5 ANSWER 152 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 67162-67-8 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl-8-(4-methyl-1-piperazinyl)-, monohydrobromide (9CI) (CA INDEX NAME)
MF C12 H18 N6 O2 . Br H
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)
CRN (67162-66-7)

Searched by: Mary Hale 308-4258 CM-1 12D16



● HBr

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:109376 Piperazine derivatives of dimethylxanthines. V. Preparation and properties of 8-piperazino- and 1-.beta.-hydroxypropyl-8-piperazinotheobromines. Cygankiewicz, Andrzej; Gorczyca, Maria; Zejc, Alfred; Zimon, Romuald (Dep. Pharm. Chem., Sch. Med., Krakow, Pol.). Acta Pol. Pharm., 34(6), 607-12 (Polish) 1977. CODEN: APPHAX. ISSN: 0001-6837.

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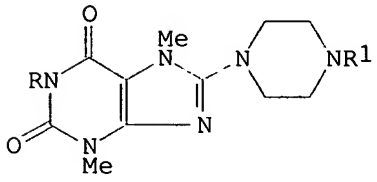
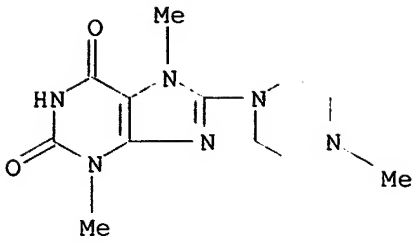


I, R=H
II, R=$CH_2CH(OH)Me$

AB 8-Bromotheobromine and anhyd. piperazine heated in MeOCH2CH2OH gave 67% I (R1 = H). I [R1 = Me, CH2CH2OH, and CH2CH(OH)Me] were prepd. analogously in 68-72% yields. I heated in PrOH with 2,3-epoxypropane in presence of pyridine gave 48-75% II [R1 = H, Me, CH2CH(OH)Me], which were also obtained in the reaction of 1-(.beta.-hydroxypropyl)-8-bromotheobromine with the appropriately substituted piperazine. All I and II were characterized as HCl or HBr salts, and most of the hydroxylated I and II, also as the Ac derivs. I and II were synthesized as potential spasmolytics and antihistaminics.

L5 ANSWER 153 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 67162-66-7 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl-8-(4-methyl-1-piperazinyl)-(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H18 N6 O2
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS, CHEMCATS
(*File contains numerically searchable property data)

Searched by: Mary Hale 308-4258 CM-1 12D16

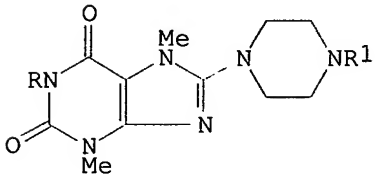


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:109376 Piperazine derivatives of dimethylxanthines. V. Preparation and properties of 8-piperazino- and 1-.beta.-hydroxypropyl-8-piperazinotheobromines. Cygankiewicz, Andrzej; Gorczyca, Maria; Zejc, Alfred; Zimon, Romuald (Dep. Pharm. Chem., Sch. Med., Krakow, Pol.). Acta Pol. Pharm., 34(6), 607-12 (Polish) 1977. CODEN: APPHAX. ISSN: 0001-6837.

GI

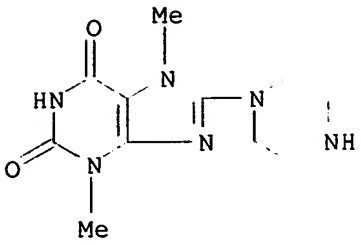


I, R=H
II, R=$CH_2CH(OH)Me$

AB 8-Bromotheobromine and anhyd. piperazine heated in MeOCH2CH2OH gave 67% I (R1 = H). I [R1 = Me, CH2CH2OH, and CH2CH(OH)Me] were prepd. analogously in 68-72% yields. I heated in PrOH with 2,3-epoxypropane in presence of pyridine gave 48-75% II [R1 = H, Me, CH2CH(OH)Me], which were also obtained in the reaction of 1-(.beta.-hydroxypropyl)-8-bromotheobromine with the appropriately substituted piperazine. All I and II were characterized as HCl or HBr salts, and most of the hydroxylated I and II, also as the Ac derivs. I and II were synthesized as potential spasmolytics and antihistaminics.

L5 ANSWER 154 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 67162-65-6 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl-8-(1-piperazinyl)-, dihydrochloride (9CI) (CA INDEX NAME)
MF C11 H16 N6 O2 . 2 Cl H
LC STN Files: CA, CAPLUS
CRN (67162-64-5)

Searched by: Mary Hale 308-4258 CM-1 12D16

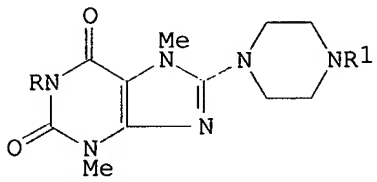


●2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:109376 Piperazine derivatives of dimethylxanthines. V. Preparation and properties of 8-piperazino- and 1-.beta.-hydroxypropyl-8-piperazinotheobromines. Cygankiewicz, Andrzej; Gorczyca, Maria; Zejc, Alfred; Zimon, Romuald (Dep. Pharm. Chem., Sch. Med., Krakow, Pol.). Acta Pol. Pharm., 34(6), 607-12 (Polish) 1977. CODEN: APPHAX. ISSN: 0001-6837.

GI

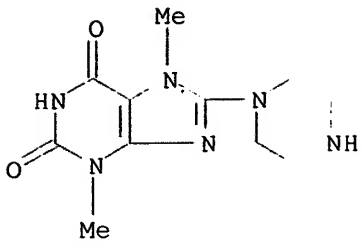


I, R=H
II, R=$CH_2CH(OH)Me$

AB 8-Bromotheobromine and anhyd. piperazine heated in MeOCH2CH2OH gave 67% I (R1 = H). I [R1 = Me, CH2CH2OH, and CH2CH(OH)Me] were prepd. analogously in 68-72% yields. I heated in PrOH with 2,3-epoxypropane in presence of pyridine gave 48-75% II [R1 = H, Me, CH2CH(OH)Me], which were also obtained in the reaction of 1-(.beta.-hydroxypropyl)-8-bromotheobromine with the appropriately substituted piperazine. All I and II were characterized as HCl or HBr salts, and most of the hydroxylated I and II, also as the Ac derivs. I and II were synthesized as potential spasmolytics and antihistaminics.

L5 ANSWER 155 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 67162-64-5 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C11 H16 N6 O2
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS, CHEMCATS
(*File contains numerically searchable property data)

Searched by: Mary Hale 308-4258 CM-1 12D16

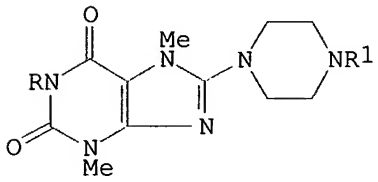


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:109376 Piperazine derivatives of dimethylxanthines. V. Preparation and properties of 8-piperazino- and 1-.beta.-hydroxypropyl-8-piperazinotheobromines. Cygankiewicz, Andrzej; Gorczyca, Maria; Zejc, Alfred; Zimon, Romuald (Dep. Pharm. Chem., Sch. Med., Krakow, Pol.). Acta Pol. Pharm., 34(6), 607-12 (Polish) 1977. CODEN: APPHAX. ISSN: 0001-6837.

GI



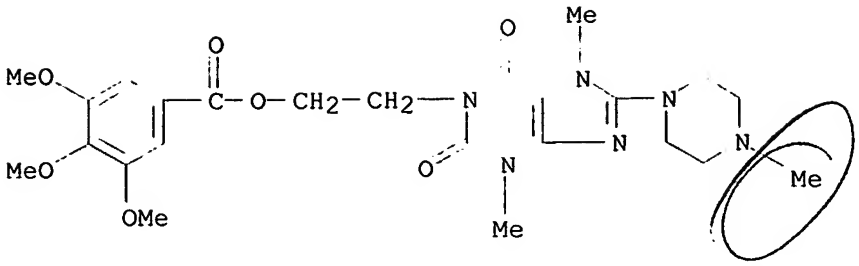
I, R=H

II, R=$CH_2CH(OH)Me$

AB 8-Bromotheobromine and anhyd. piperazine heated in MeOCH2CH2OH gave 67% I (R1 = H). I [R1 = Me, CH2CH2OH, and CH2CH(OH)Me] were prepd. analogously in 68-72% yields. I heated in PrOH with 2,3-epoxypropane in presence of pyridine gave 48-75% II [R1 = H, Me, CH2CH(OH)Me], which were also obtained in the reaction of 1-(.beta.-hydroxypropyl)-8-bromotheobromine with the appropriately substituted piperazine. All I and II were characterized as HCl or HBr salts, and most of the hydroxylated I and II, also as the Ac derivs. I and II were synthesized as potential spasmolytics and antihistaminics.

L5 ANSWER 156 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 62164-84-5 REGISTRY
CN Benzoic acid, 3,4,5-trimethoxy-, 2-[2,3,6,7-tetrahydro-3,7-dimethyl-8-(4-methyl-1-piperazinyl)-2,6-dioxo-1H-purin-1-yl]ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H32 N6 O7
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:139992 1,8-Disubstituted derivatives of theobromine and their pharmacological activity. Gutorov, L. A.; Ovcharova, I. M.; Golovchinskaya, E. S.; Muratov, M. A.; Kaminka, M. E.; Mashkovskii, M. D. (Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR). Khim.-Farm. Zh., 10(12), 61-4 (Russian) 1976. CODEN: KHFZAN.

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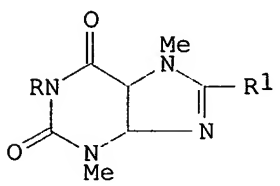
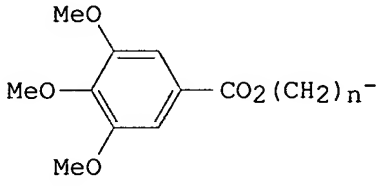


I

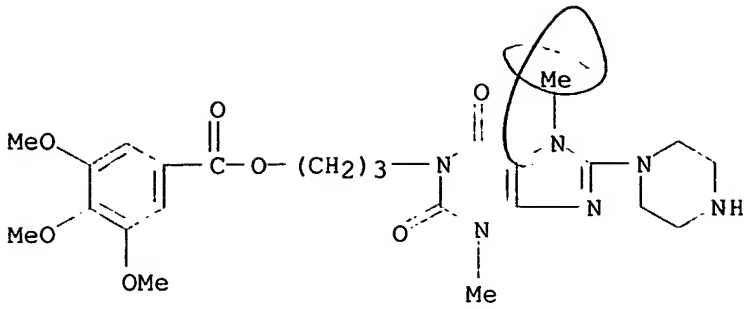


II, n=2,3

AB Theobromine derivs. I (R = II, R1 = Et2NCH2) were obtained in 68.5 and 71.7% yields by heating I (R = H) with chloroalkyl 3,4,5-trimethoxybenzoates. Analogous alkylation of I (R = H, R1 = Cl) gave 70.4 and 42.2% I (R = II, R1 = Cl) which were aminated by piperazine derivs. to give 78.2-84.5% I (R = II, R1 = 1-piperazinyl, 4-methyl-1-piperazinyl). Alkylation of the latter with Cl(CH2)nOH (n = 2,3), and ClCH2CH(OH)CH2OH gave 40.5-70.4% of the hydroxyalkylpiperazinyl theobromine derivs. I were useful as broncholytics, vasodilators, and as antihypertensives.

L5 ANSWER 157 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 62128-72-7 REGISTRY
CN Benzoic acid, 3,4,5-trimethoxy-, 3-[2,3,6,7-tetrahydro-3,7-dimethyl-2,6-dioxo-8-(1-piperazinyl)-1H-purin-1-yl]propyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H32 N6 O7
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Searched by: Mary Hale 308-4258 CM-1 12D16

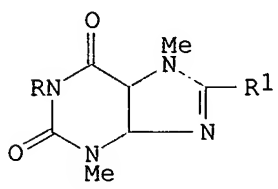


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:139992 1,8-Disubstituted derivatives of theobromine and their pharmacological activity. Gutorov, L. A.; Ovcharova, I. M.; Golovchinskaya, E. S.; Muratov, M. A.; Kaminka, M. E.; Mashkovskii, M. D. (Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR). Khim.-Farm. Zh., 10(12), 61-4 (Russian) 1976. CODEN: KHFZAN.

GI



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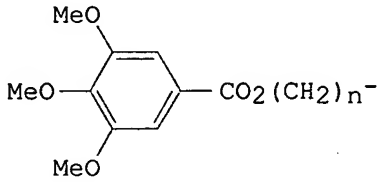
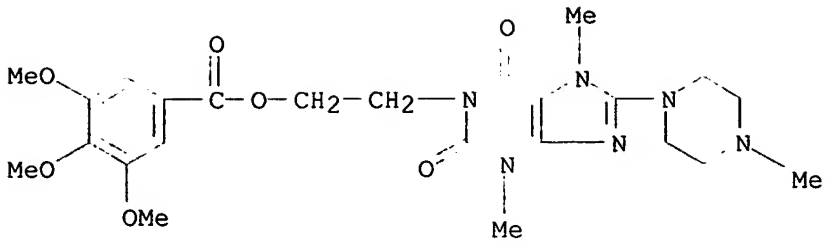


II, n=2,3

AB Theobromine derivs. I (R = II, R1 = Et2NCH2) were obtained in 68.5 and 71.7% yields by heating I (R = H) with chloroalkyl 3,4,5-trimethoxybenzoates. Analogous alkylation of I (R = H, R1 = Cl) gave 70.4 and 42.2% I (R = II, R1 = Cl) which were aminated by piperazine derivs. to give 78.2-84.5% I (R = II, R1 = 1-piperazinyl, 4-methyl-1-piperazinyl). Alkylation of the latter with Cl(CH2)nOH (n = 2,3), and ClCH2CH(OH)CH2OH gave 40.5-70.4% of the hydroxyalkylpiperazinyl theobromine derivs. I were useful as broncholytics, vasodilators, and as antihypertensives.

L5 ANSWER 158 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 62128-71-6 REGISTRY
CN Benzoic acid, 3,4,5-trimethoxy-, 2-[2,3,6,7-tetrahydro-3,7-dimethyl-8-(4-methyl-1-piperazinyl)-2,6-dioxo-1H-purin-1-yl]ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)
MF C24 H32 N6 O7 . Cl H
LC STN Files: CA, CAPLUS
CRN (62164-84-5)

Searched by: Mary Hale 308-4258 CM-1 12D16

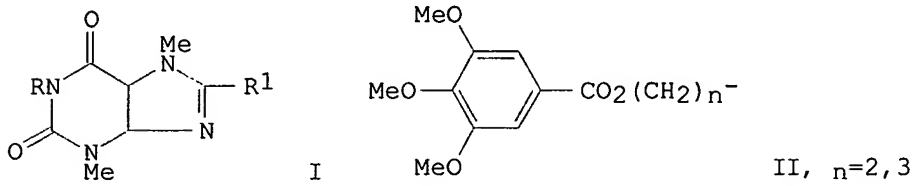


● HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:139992 1,8-Disubstituted derivatives of theobromine and their pharmacological activity. Gutorov, L. A.; Ovcharova, I. M.; Golovchinskaya, E. S.; Muratov, M. A.; Kaminka, M. E.; Mashkovskii, M. D. (Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR). Khim.-Farm. Zh., 10(12), 61-4 (Russian) 1976. CODEN: KHFZAN.

GI

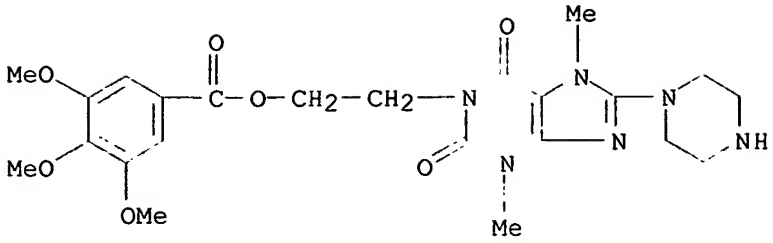


I II, n=2,3

AB Theobromine derivs. I (R = II, R1 = Et2NCH2) were obtained in 68.5 and 71.7% yields by heating I (R = H) with chloroalkyl 3,4,5-trimethoxybenzoates. Analogous alkylation of I (R = H, R1 = Cl) gave 70.4 and 42.2% I (R = II, R1 = Cl) which were aminated by piperazine derivs. to give 78.2-84.5% I (R = II, R1 = 1-piperazinyl, 4-methyl-1-piperazinyl). Alkylation of the latter with Cl(CH2)nOH (n = 2,3), and ClCH2CH(OH)CH2OH gave 40.5-70.4% of the hydroxyalkylpiperazinyl theobromine derivs. I were useful as broncholytics, vasodilators, and as antihypertensives.

L5 ANSWER 159 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 62128-70-5 REGISTRY
CN Benzoic acid, 3,4,5-trimethoxy-, 2-[2,3,6,7-tetrahydro-3,7-dimethyl-2,6-dioxo-8-(1-piperazinyl)-1H-purin-1-yl]ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)
MF C23 H30 N6 O7 . Cl H
LC STN Files: CA, CAPLUS, CHEMCATS
CRN (62128-69-2)

Searched by: Mary Hale 308-4258 CM-1 12D16



● HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:139992 1,8-Disubstituted derivatives of theobromine and their pharmacological activity. Gutorov, L. A.; Ovcharova, I. M.; Golovchinskaya, E. S.; Muratov, M. A.; Kaminka, M. E.; Mashkovskii, M. D. (Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR). Khim.-Farm. Zh., 10(12), 61-4 (Russian) 1976. CODEN: KHFZAN.

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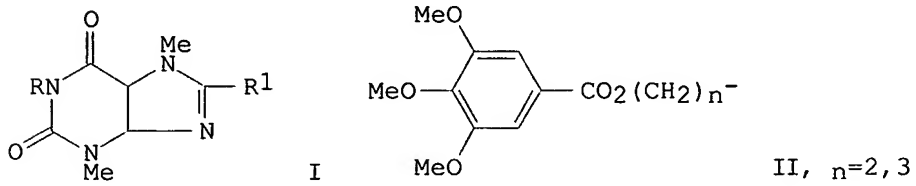
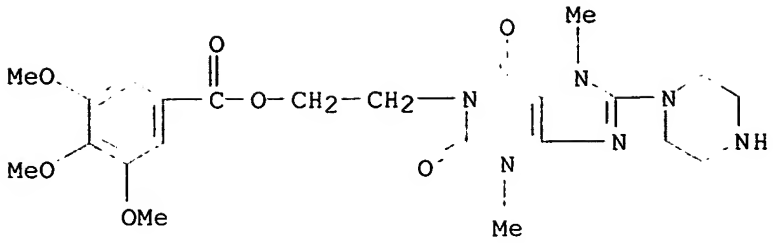


I II, n=2,3

AB Theobromine derivs. I (R = II, R1 = Et2NCH2) were obtained in 68.5 and 71.7% yields by heating I (R = H) with chloroalkyl 3,4,5-trimethoxybenzoates. Analogous alkylation of I (R = H, R1 = Cl) gave 70.4 and 42.2% I (R = II, R1 = Cl) which were aminated by piperazine derivs. to give 78.2-84.5% I (R = II, R1 = 1-piperazinyl, 4-methyl-1-piperazinyl). Alkylation of the latter with Cl(CH2)nOH (n = 2,3), and ClCH2CH(OH)CH2OH gave 40.5-70.4% of the hydroxyalkylpiperazinyl theobromine derivs. I were useful as broncholytics, vasodilators, and as antihypertensives.

L5 ANSWER 160 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 62128-69-2 REGISTRY
CN Benzoic acid, 3,4,5-trimethoxy-, 2-[2,3,6,7-tetrahydro-3,7-dimethyl-2,6-dioxo-8-(1-piperazinyl)-1H-purin-1-yl]ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H30 N6 O7
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS, CHEMCATS
(*File contains numerically searchable property data)

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:139992 1,8-Disubstituted derivatives of theobromine and their pharmacological activity. Gutorov, L. A.; Ovcharova, I. M.; Golovchinskaya, E. S.; Muratov, M. A.; Kaminka, M. E.; Mashkovskii, M. D. (Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR). Khim.-Farm. Zh., 10(12), 61-4 (Russian) 1976. CODEN: KHFZAN.

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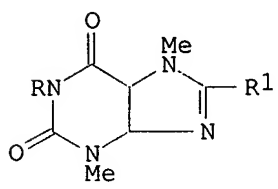
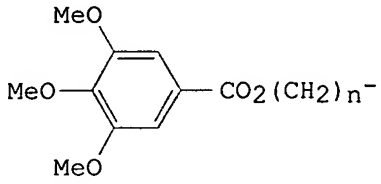


I

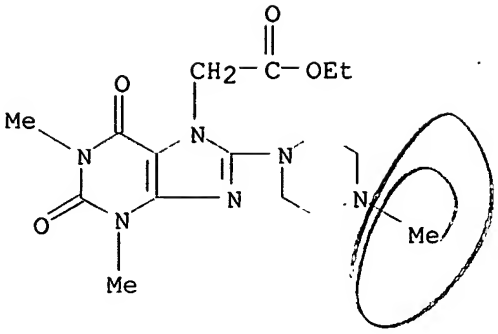


II, n=2,3

AB Theobromine derivs. I (R = II, R1 = Et2NCH2) were obtained in 68.5 and 71.7% yields by heating I (R = H) with chloroalkyl 3,4,5-trimethoxybenzoates. Analogous alkylation of I (R = H, R1 = Cl) gave 70.4 and 42.2% I (R = II, R1 = Cl) which were aminated by piperazine derivs. to give 78.2-84.5% I (R = II, R1 = 1-piperazinyl, 4-methyl-1-piperazinyl). Alkylation of the latter with Cl(CH2)nOH (n = 2,3), and ClCH2CH(OH)CH2OH gave 40.5-70.4% of the hydroxyalkylpiperazinyl theobromine derivs. I were useful as broncholytics, vasodilators, and as antihypertensives.

L5 ANSWER 161 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 52943-70-1 REGISTRY
CN 7H-Purine-7-acetic acid, 1,2,3,6-tetrahydro-1,3-dimethyl-8-(4-methyl-1-piperazinyl)-2,6-dioxo-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H24 N6 O4
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Searched by: Mary Hale 308-4258 CM-1 12D16



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

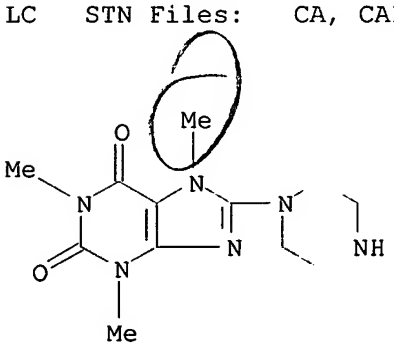
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 81:37537 Substitution derivatives of theophylline at the 7 and 8 positions. Lespagnol, Albert; Van Aerde, Christine (Lab. Pharm. Chim., Fac. Pharm., Lille, Fr.). C. R. Acad. Sci., Ser. C, 278(18), 1145-7 (French) 1974. CODEN: CHDCAQ.

GI For diagram(s), see printed CA Issue.

AB Theophyllines I [R = H, CH2CO2Et; R1 = [(3-phenothiazin-5-ylpropyl)amino], N-methylpiperazino, PhOCH2CH2NH, Ph2CHNH, (PhCH2)2N, PhCH2(PhCH2CH2)N] were prepd. by treating I (R1 = Br) with the amine. Reaction of I (R = CH2CO2Et, R1 = Br) with H2NCHPh2 also gave I (R = CH2CONHCHPh2, R1 = NHCHPh2). The reaction of I (R = H, R1 = Br) with pyridine gave the ylide II and hydrated derivs., both isolable. The phenothiazinylpropylamines III (R2 = H, Cl, CF3, OMe; R3 = (CH2)3NH2) were prepd. by cyanoethylating III (R3 = H) and reducing the resulting III (R3 = CH2CH2CN).

L5 ANSWER 162 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 50693-74-8 REGISTRY
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-8-(1-piperazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H18 N6 O2
LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:351159 Synthesis of 8-substituted xanthines and their oxidative skeleton rearrangement to 1-oxo-2,4,7,9-tetraazaspiro[4,5]dec-2-

Searched by: Mary Hale 308-4258 CM-1 12D16

ene-6,8,10-triones. Zimmer, Hans; Amer, Adel; Baumann, Frank M.; Haecker, Michael; Hess, Christopher G. M.; Ho, Douglas; Huber, Hans J.; Koch, Klaus; Mahnke, K.; Schumacher, Christian; Wingfield, Robert C. (Dep. Chemistry, Univ. Cincinnati, Cincinnati, OH, 45221, USA). Eur. J. Org. Chem. (9), 2419-2428 (English) 1999. CODEN: EJOCFK. ISSN: 1434-193X. Publisher: Wiley-VCH Verlag GmbH.

AB The synthesis of a no. of 8-(dialkylamino)xanthines- and 8-alkoxyxanthines is described. Treatment of 8-(dialkylamino)xanthines with 3-ClC6H4CO3H (m-CPBA) gave 3-(dialkylamino)-4,7,9-trimethyl-1-oxo-2,4,7,9-tetraazaspiro[4,5]dec-2-ene-6,8,10-triones by a novel rearrangement. Also, the corresponding 3-alkoxylated spiro compds. were obtained by an analogous treatment of 8-alkoxyxanthines. In attempts to elucidate a tentative mechanism for this rearrangement, 8-[(dialkylamino)methyl]caffeines on treatment with m-CPBA did not undergo the rearrangement but only yielded the expected N-oxides. This result seems to indicate that a necessary structure element for this rearrangement to occur is an atom with an unshared pair of electrons to be attached to the 8-position of the investigated xanthines. In agreement with this statement is the fact that N-oxides of 8-[(dialkylamino)methyl]caffeines do not undergo the novel rearrangement but rather give the expected Meisenheimer rearrangement or the Cope elimination depending upon reaction conditions.

REFERENCE 2: 80:3493 Antitussive oxazolinylpiperazines. Goebel, Axel; Schmitt, Karl; Linde-Ranke, Ida (Farbwerke Hoechst A.-G.). Ger. Offen. DE 2205815 19730816, 19 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1972-2205815 19720208.

GI For diagram(s), see printed CA Issue.

AB Fifty-five piperazines [I; R = Bu, CH2CHMe2, CH2CO2Et, Ph, substituted phenyl, or a heterocyclic group, e.g. 2-pyridyl or 2-quinolyl; R1 = Me, CH2Cl, or CH:CH2, R2 and R3 = H or Me, or R2R3 = (CH2)3 or (CH2)6], useful as antitussives, were prepd. as hydrobromides by reaction of II with OCNCR1R2CHR3Br. I (R = 2-MeC6H4, R1-R3 = H) was prepd. by reaction of II (R = 2-MeC6H4) with OCNCH2CH2Cl or successively with COCl2 and ethylenimine. I.HBr (R = 2,4-ClMeC6H3, R1 = Me, R2 = R3 = H) had LD50 560 mg/kg orally in mice and antitussive effect in 0.25 mg/kg doses i.v. in cats.

L5 ANSWER 163 OF 168 REGISTRY COPYRIGHT 2002 ACS

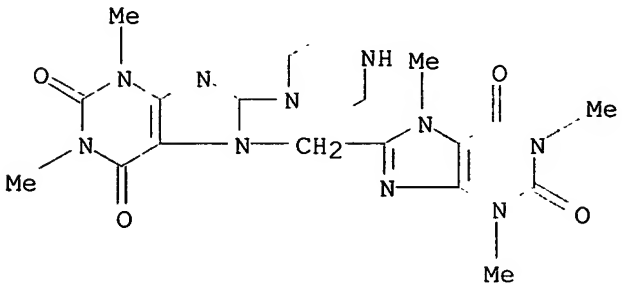
RN 25472-93-9 REGISTRY

CN Caffeine, 8-[[1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-8-(1-piperazinyl)purin-7-yl]methyl]- (8CI) (CA INDEX NAME)

FS 3D CONCORD

MF C20 H26 N10 O4

LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Searched by: Mary Hale 308-4258 CM-1 12D16

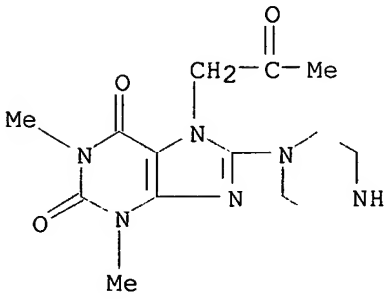
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 72:55410 Synthesis of substituted bisxanthines. Kleine, K. H.; Graefe, Guenter; Haller, Rolf (Pharm. Inst., Univ. Freiburg/Br., Freiburg/Br., Ger.). Arzneim.-Forsch., 19(11), 1854-5 (German) 1969. CODEN: ARZNAD.

GI For diagram(s), see printed CA Issue.

AB I (R = Br) (3.3 millimoles) was treated with 33 millimoles piperidine in 15 ml EtOH 13 hr at 140-5.degree. to give 72% I (R = piperidino), m. 176-8.degree.. The following compds. were similarly prepd. (compd., R, % yield, and m.p. given): I, morpholino, 75, 208-10.degree.; I, NEt2, 86, 130-1.degree.; I, iso-PrNH, 88, 188-90.degree.; I, NHCH2CH2OH, 96, 219-21.degree.; II, piperidino, 99, 265-6.degree. (decompn.); II, 1-piperazinyl, 100, 250-2.degree. (decompn.); II, 4-(2-hydroxyethyl)-1-piperazinyl, 94, 279-80.degree.. I (R = Br) (4 g) was refluxed with 4.53 g NaSH in 120 ml 80% iso-PrOH 2 hr to give 69% I (R = SH), m. 190-2.degree. (decompn.), which on treatment with NaOAc-MeI gave 82% I (R = SMe), m. 258-9.degree.. I (R = SEt), m. 188-9.degree. (decompn.), was similarly prepd. in 72% yield.

L5 ANSWER 164 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 24961-90-8 REGISTRY
CN Theophylline, 7-acetonyl-8-(1-piperazinyl)-, monohydrochloride (8CI) (CA INDEX NAME)
MF C14 H20 N6 O3 . Cl H
LC STN Files: CA, CAPLUS, TOXCENTER, TOXLIT
CRN (24961-80-6)



● HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 71:59504 Pharmacological studies of basic theophylline derivatives. II. Toxicity and effects on tracheal smooth muscle and histamine release. Kubota, Kazuhiko; Kono, Shigeharu; Koreeda, Tadako (Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, Japan). Yakugaku Zasshi, 89(4), 446-9 (Japanese) 1969. CODEN: YKKZAJ.

AB Theophylline derivs. (Kubota, et al., 1969) were evaluated for anti-histaminic effects on tracheal smooth muscles excised from guinea pigs. None of them exceeded theophylline in antihistaminic activity, but incorporation of the basic polar groups lowered the acute toxicity with min. loss of the activity. A theophylline deriv. with 7-acetonyl and 8-piperazino substituents exhibited a histamine-releasing action, as

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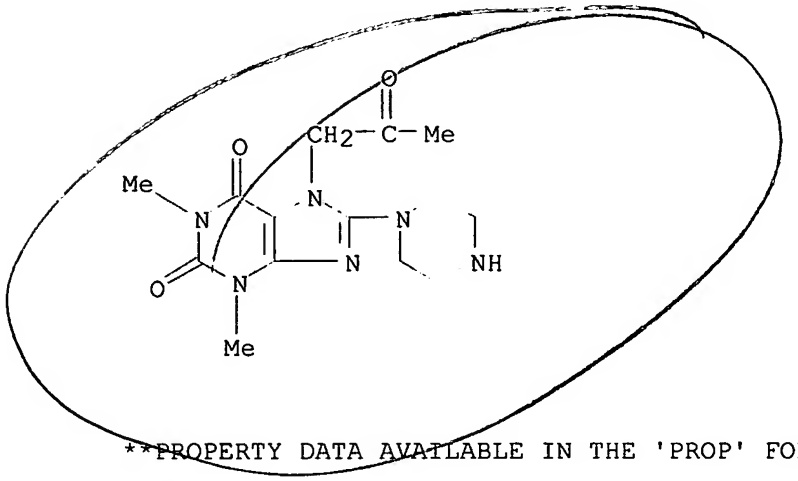
examd. with rat mast cells and rat paw edema.

L5 ANSWER 165 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 24961-80-6 REGISTRY
CN Theophylline, 7-acetonyl-8-(1-piperazinyl)- (8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H20 N6 O3
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXLIT
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 71:59503 Pharmacological studies of basic theophylline derivatives. I. Effects on the cardiovascular system. Kubota, Kazuhiko; Kono, Shigeharu; Koreeda, Tadako (Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, Japan). Yakugaku Zasshi, 89(4), 441-5 (Japanese) 1969. CODEN: YKKZAJ.
GI For diagram(s), see printed CA Issue.
AB The following new theophylline (I) derivs. were evaluated for their cardiovascular effects on dogs (7- and 8-substituents and m.p. given): CH2CH2C(:NOH)NH2, H, 203-5.degree.; CH2C(:NOH)NH2, H, 227-30.degree.; CH2Ac, piperazino, 192.degree.; CH2Ac, morpholino, 167.degree.. Also tested were II (R, R1, and m.p. given): Bu, H, 93.degree.; Et, Et, 85.degree.; (RR1 =) piperidino, 158.degree.; (RR1 =) morpholino, 178.degree.; (RR1 =) pyrrolidino, 112.degree.; and III (R2 and m.p. given): piperidino, 202.degree.; Et2N, 160.degree. (IV). Most of the compds. increased the blood flow of renal, femoral, and internal carotid arteries, but the effect was of the order of that of I. IV, however, was 6-fold as effective in the internal carotid blood flow. In general, addn. of basic polar groups to I lessened the cardiovascular effects.

L5 ANSWER 166 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 20367-10-6 REGISTRY
CN Benzoic acid, 3,4,5-trimethoxy-, ester with 7-(2-hydroxyethyl)-8-(1-piperazinyl)theophylline (8CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Theophylline, 7-(2-hydroxyethyl)-8-(1-piperazinyl)-, 3,4,5-trimethoxybenzoate (ester)
FS 3D CONCORD
MF C23 H30 N6 O7
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB
(*File contains numerically searchable property data)

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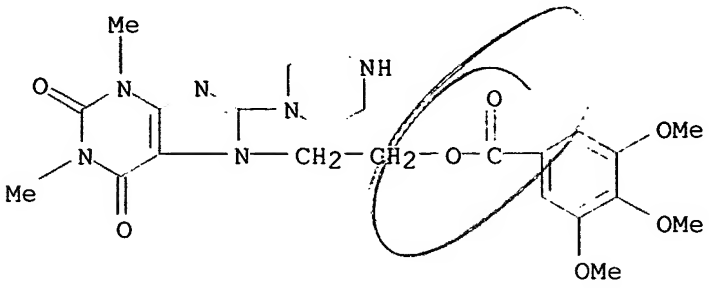

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 69:87022 Theophylline derivatives. Stachel, Adolf; Nitz, Rolf E.; Resag, Klaus; Kreiskott, Horst (Cassella Farbwerke Mainkur A.-G.). U.S. US 3399195 19680827, 4 pp. (English). CODEN: USXXAM. PRIORITY: DE 1967-C39516 19670628.

GI For diagram(s), see printed CA Issue.

AB The title compds. are effective coronary dilators and in addn. possess central nervous system depressor activity. They are prepd. by 3 different methods. Thus, a mixt. of 52 g. 8-bromotheophylline and 57.6 g. 3,4,5-(MeO)3C6H2(CH2)3Cl was stirred for 24 hrs. at 100.degree. while adding 27.6 g. K2CO3 in 150 cc. HCONMe2 to yield 100 g. 7-[3-(3,4,5-trimethoxybenzoxy)propyl]-8-bromotheophylline (I), m. 175.degree. (MePh). A soln. of 51 g. I in 250 cc. PhCl was mixed with 10.6 g. Na2CO3, a soln. of 13 g. N-(2-hydroxyethyl)piperazine in 100 cc. PhCl added dropwise at 50-60.degree. during 1 hr., and the mixt. stirred and refluxed for 12 hrs. to give 48 g. II [n = 3, A = (CH2)2, R = 3,4,5-(MeO)3, X = OH] (III), m. 130.degree. (AcOEt) [HCl salt m. 204.degree. (decompn.)]. Also described are the following II (n, AX, R, and m.p. given): 3, (CH2)3OH, 3,4,5-(MeO)3, 150.degree.; 3, CH2CHMeOH, 3,4,5-(MeO)3, 147.degree.; 3, CH2CH(OH)CH2OMe, 3,4,5-(MeO)3, 129.degree.; 3, (CH2)4, 3,4,5-(MeO)3, 141.degree.; 2, CH2CH2OH, 3,4,5-(MeO)3, 140.degree.; 2, (CH2)3OH, 3,4,5-(MeO)3, 130.degree.; 2, CH2CHMeOH, 3,4,5-(MeO)3, 115.degree.; 2, (CH2)4OH, 3,4,5-(MeO)3, 128.degree.; 2, CH2CH(OH)CH2OMe, 3,4,5-(MeO)3, 106.degree.; 2, CH2CHMeOH, 3,5-(MeO)2, 168.degree.; 2, (CH2)3OH, 3,5-(MeO)2, 166.degree.; 3, (CH2)3OH, 4-OMe, 123.degree.. To a mixt. of 28.7 g. III and 5.3 g. Na2CO3 in 200 cc. C6H6 was added at room temp. a soln. of 11.5 g. 3,4,5-(MeO)3C6H2COCl (IV) in 100 cc. C6H6, and the mixt. stirred for 1-2 hrs. and then refluxed for 3-4 hrs. to yield 25 g. HCl salt of V [n = 3, A = (CH2)2, R1 = R2 = 3,4,5-(MeO)3], m. 231.degree. (decompn.). A mixt. of 40 g. piperazine, 16 g. Na2CO3, and 75.5 g. 7-[2-(3,4,5-trimethoxybenzoxy)ethyl]-8-bromotheophylline in 300 cc. PhCl was refluxed for 24 hrs. to give II [n = 2, AX = H, R = 3,4,5-(MeO)3] (VI), m. 167-9.degree. (AcOEt). A mixt. of 50.2 g. VI, 13.8 g. K2CO3, and 29 g. 3,4,5-(MeO)3C6H2CO2(CH2)3Cl in 200 cc. HCONMe2 was stirred for 12 hrs. at 100.degree. to yield 53 g. HCl salt of V [n = 2, A = (CH2)3, R1 = R2 = 3,4,5-(MeO)3], m. 140-3.degree. (decompn.). A soln. of 46 g. IV in 100 cc. C6H6 was added dropwise to a soln. of 38 g. VII and 20.2 g. Et3N in 300 cc. C6H6, the reaction mixt. stirred for 3-4 hrs. at room temp. and refluxed for 2 hrs. to give 40 g. HCl salt of V [n = 3, A = CH2CHMe, R1 = R2 = 3,4,5-(MeO)3], m. 125.degree. (decompn.). Also described are the following V (n, A, R1, R2, and decompn. point of HCl salt given): 3, (CH2)3, 3,4,5-(MeO)3, 3,4,5-(MeO)3, 188.degree.; 3, CH2CH[O2CC6H2(OMe)3-3,4,5]CH2OMe, 3,4,5-(MeO)3, 3,4,5-(MeO)3, 95.degree.; 2, (CH2)2, 3,4,5-(MeO)3, 3,4,5-(MeO)3,

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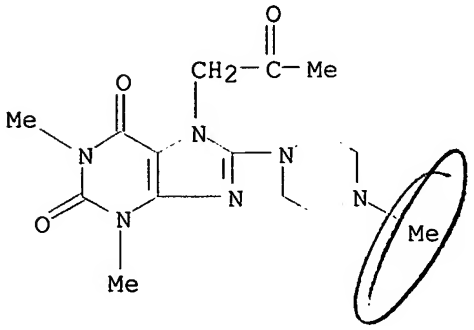
105.degree.; 2, (CH2)4, 3,4,5-(MeO)3, 3,4,5-(MeO)3, 165.degree.; 2, CH2CHMe, 3,5-(MeO)2, 3,4,5-(MeO)3, 115.degree.; 2, (CH2)3, 3,5-(MeO)2, 3,5-(MeO)2, 123.degree.; 3, (CH2)3, 4-MeO, 3,4,5-(MeO)3, 107.degree.; 3, (CH2)4, 3,4,5-(MeO)3, 3,4,5-(MeO)3, 123.degree.; 2, CH2CHMe, 3,4,5-(OMe)3, 115.degree.; 2, CH2CH[O2CC6H2(OMe)3-3,4,5]CH2OMe, 3,4,5-(MeO)3, 3,4,5-(MeO)3, 113.degree..

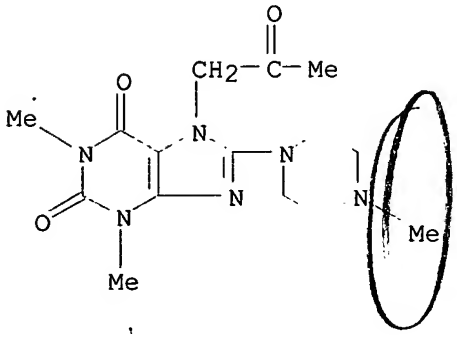
L5 ANSWER 167 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 903-54-8 REGISTRY
CN Theophylline, 7-acetonyl-8-(4-methyl-1-piperazinyl)-, monohydrochloride (8CI) (CA INDEX NAME)
MF C15 H22 N6 O3 . Cl H
LC STN Files: CAOLD
CRN (743-53-3)



● HCl

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L5 ANSWER 168 OF 168 REGISTRY COPYRIGHT 2002 ACS
RN 743-53-3 REGISTRY
CN Theophylline, 7-acetonyl-8-(4-methyl-1-piperazinyl)- (7CI, 8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H22 N6 O3
CI COM
LC STN Files: BEILSTEIN*, CAOLD
(*File contains numerically searchable property data)



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Searched by: Mary Hale 308-4258 CM-1 12D16

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	619.54	1851.42

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-18.29	-73.04

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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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L6 5 L5

=> d 1-5

L6 ANSWER 1 OF 5 CAOLD COPYRIGHT 2002 ACS
AN CA62:9130d CAOLD
TI purine azides
AU Smirnova, N. B.; Postovskii, I. Ya.
IT 75-98-9 **743-53-3** **903-54-8** 910-46-3
910-47-4 975-43-9 975-44-0 977-76-4 977-77-5 979-51-1
979-52-2 979-53-3 1051-14-5 1051-15-6 1051-26-9 7029-99-4
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L6 ANSWER 2 OF 5 CAOLD COPYRIGHT 2002 ACS
AN CA59:1658g CAOLD
TI pyrazolo[2,3-a]pyrimidine derivs.
AU Takamizawa, Akira; Hayashi, S.
PA Shionogi & Co., Ltd.
DT Patent

PATENT NO.	KIND	DATE
JP 62005191		1962

IT 90090-71-4 90559-16-3 91337-94-9 97361-17-6 97619-27-7
97725-83-2 98147-52-5 98964-20-6 100412-13-3 101201-75-6
106571-85-1

L6 ANSWER 3 OF 5 CAOLD COPYRIGHT 2002 ACS
AN CA58:5670g CAOLD
TI caffeine-8-alkylene diamines
AU Klosa, Josef

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